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http://www.aps.org/meetings/march/index.cfm
surprising soft behavior with temperature changes: its energy increases with temperature and reaches the Zeeman energy for temperatures above 2K. These experiments [2] have suggested the possibility of observing a long range Skyrme crystal phase with non-collinear magnetic order at low temperatures. The magnetic properties of the 2DES close to \( \nu = 1 \) are studied by the direct measurement of the low-lying spin wave excitations by inelastic light scattering between 2.5K and 40mK. We discovered a very low energy spin wave that emerges on both sides of \( \nu = 1 \). The spin wave is well below the Zeeman energy and exhibit surprising soft behavior with temperature changes: its energy increases with temperature and reaches the Zeeman energy for temperatures above 2K. These results suggest an instability of the 2DES towards magnetic order at low temperatures and filling factors close to \( \nu = 1 \). The spin excitation spectra are consistent with the ordering of the in-plane components of spin in a square Skyrme crystal phase proposed in theoretical evaluations [3], but never fully confirmed by experiments. Our experiments create venues for the determination of Skyrme crystal phases from measurements of low-lying spin excitations by inelastic light scattering.

Supported by NSF Grant No. NMR-0352738 and by DOE Grant No. DE-AIO2-04ER46133.

Work performed at Columbia University (USA) in collaboration with J.Yan, A.Pinczuk, L.N. Pfeiffer and K.W.West.

8:36AM A1.00002 Soft spin waves and magnetic instability in Skyrmion systems\(^1\), YANN GALLAIS\(^2\).

Universite Paris 7 — In this work the highly correlated ground states of spin in 2D electron layers (2DES) near filling factor \( \nu = 1 \) are probed by inelastic light scattering [1]. In this filling factor region the ground state of the 2DES is affected by the proliferation of spin-charge textures known as Skyrmions. Recent experiments [2] have suggested the possibility of observing a long range Skyrmion crystal phase with non-collinear magnetic order at low temperatures. The magnetic properties of the 2DES close to \( \nu = 1 \) are studied by the direct measurement of the low-lying spin wave excitations by inelastic light scattering between 2.5K and 40mK. We discovered a very low energy spin wave that emerges on both sides of \( \nu = 1 \). The spin wave is well below the Zeeman energy and exhibit surprising soft behavior with temperature changes: its energy increases with temperature and reaches the Zeeman energy for temperatures above 2K. These results suggest an instability of the 2DES towards magnetic order at low temperatures and filling factors close to \( \nu = 1 \). The spin excitation spectra are consistent with the ordering of the in-plane components of spin in a square Skyrmion crystal phase proposed in theoretical evaluations [3], but never fully confirmed by experiments. Our experiments create venues for the determination of Skyrmion crystal phases from measurements of low-lying spin excitations by inelastic light scattering.

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9:12AM A1.00003 High Resolution Spectroscopy of the Quantum Hall Liquid, OLIVER DIAL.

Massachusetts Institute of Technology — We present precise and unprecedentedly high resolution spectra of the tunneling density of states (TDOS) of a cold two dimensional electron system (2DES) in GaAs over an energy range from 15 meV above to 15 meV below the Fermi surface. The results provide the first direct measurements of the width of the single-particle exchange gap and lifetimes in the quantum Hall system. At higher energies, we show the first observations of exchange-induced spin-splittings in fully filled or unfilled Landau levels not at the Fermi energy. The results demonstrate a counter-intuitive fact: the high energy spectrum reflects correlations that only appear at very low temperatures. For instance, upon raising the temperature from 100 mK (0.01 meV) to 1 K (0.1 meV) changes are seen in the spectrum at 10 meV away from the Fermi energy. Along with measurements of exchange splittings and lifetimes, we observe an unpredicted new structure appearing only at high magnetic fields and low temperatures that appears to be a long lived quasi-particle. The results are made possible by a novel technique, time domain capacitance spectroscopy. It allows us to measure the TDOS of a 2DES with resolution only limited by temperature, even at large tunneling energies. In TDCS, sharp voltage pulses disequilibrate a 2DES from a nearby metallic contact inducing a tunnel current perpendicular to the plane of the 2DES. We detect this current by monitoring the image charge of the tunneling electrons on a distant electrode. No ohmic contact to the 2DES is required. The technique works even when the 2DES is empty or has vanishing in-plane conductivity, as frequently occurs in the quantum Hall effect. Importantly, we can eliminate the effects of ohmic heating in the experiment by using short duty cycle pulses, with currents flowing only 0.01% of the time. The obtained spectra reveal the beautiful and difficult to reach structure present far from the Fermi surface in the quantum Hall system.

9:48AM A1.00004 Magnetotunneling spectroscopy: Imaging electron wavefunctions and measuring electron dispersion curves in GaMnAs- and GaAsN-based heterostructures, LAURENCE EAVES.

School of Physics and Astronomy, University of Nottingham — Magnetotunnelling spectroscopy is a powerful tool for imaging the wavefunctions of electrons in quantum wires [1] and dots [2] and for measuring the energy-wavevector dispersion curves of holes [3] and electrons [4] in novel quantum well structures. It uses the effect of the Lorentz force to tune the in-plane momentum of a tunneling electron when it enters a quantum-confined structure [4]. This talk will describe recent work to spatially image the ground and excited state wavefunction of electrons confined in quantum dots in ferromagnetic GaMnAs tunnel diodes. These dots are formed by the electrostatic potential arising from clusters of charged Mn interstitial donors. It will also be shown how the fragmented conduction electron dispersion curves of GaAsN give rise to highly non-linear electron dynamics and a new type of negative differential conductivity effect.

8:36AM A2.00002 Dichroism in the pseudogap phase observed through high precision Sagnac interferometry, ELIZABETH SCHEMM, Department of Physics, Stanford University — Polar Kerr effect in the high-\(T_c\) superconductor \(\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}\) was measured at zero magnetic field with high precision using a cryogenic Sagnac fiber interferometer. We observed non-zero Kerr rotations on the order of \(\sim 1\) \(\mu\)rad appearing near the pseudogap temperature \(T^*\), and marking what appears to be a true phase transition. Anomalous magnetic behavior in magnetic-field training of the effect suggests that other high temperature superconductors will also be discussed.

Work done in collaboration with Jing Xia and Aharon Kapitulnik.

1Work supported by Department of Energy grant DEFG03-01ER45925.

9:12AM A2.00003 Orbital-Current phases in one- and two-dimensional strongly correlated systems, THIERRY GIAMARCHI, University of Geneva — Although we now know that strongly correlated systems can have several type of conventional order ranging from charge or spin order to superconductivity, the possibility that they present also more exotic phases remains an elusive but very challenging question. In particular whether such systems can have orbital current order for realistic interactions has been strongly debated. Recently this question has come to attention again due to theoretical proposals and subsequent neutron scattering experiments suggesting that this could be the case in the pseudogap phase of High \(T_c\). Tackling this issue directly for the two dimensional case is difficult, since no uncontrolled method can be used beyond exact diagonalization for very small clusters. However this question can be looked at on the one dimensional (ladder) version of this problem, where such orbital current phases can be studied by well controlled methods such as bosonization. I will present the results we obtained on these systems and discuss in particular the comparison between the case of a simple Hubbard ladder [1] versus a three band model (\(\text{Cu-O ladder}\) [2].

In order to tackle these issues for the two-dimensional case, we have performed a variational Monte Carlo analysis for a three band Cu-O model. This technique although depending on the quality of the variational wave function has the advantage of being essentially free of numerical problems. I will discuss the phases obtained by this approach as well as the possible experimental consequences.

These works are a collaboration with E. Orignac; P. Chudzinski and M. Gabay; C. Weber, A. Laëuchli and F. Mila.


9:48AM A2.00004 Inhomogeneous Superconductivity in \(\text{YBa}_2\text{Cu}_3\text{O}_y\) and \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) Above \(T_c\), JEFF SONIER, Simon Fraser University — An exciting development in the immense research effort focused on resolving the origin of high-\(T_c\) superconductivity, is the growing evidence for signatures of superconductivity in cuprate materials at temperatures far above \(T_c\). Recent STM experiments on \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) have provided new insight into the precise nature of these pairing correlations, by revealing the occurrence of nanometre-sized pairing regions above \(T_c\). Whether nanoscale inhomogeneous superconductivity is universal to the cuprates, and whether \(T_c\) is driven by Kosterlitz- Thouless physics or Josephson coupling between nanometre-sized superconducting regions is matters of current debate. Very recently we have used \(\mu\)SR to probe the local response in the bulk of \(\text{YBa}_2\text{Cu}_3\text{O}_y\) and \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) single crystals to a large applied magnetic field (\(H = 7\) T). At temperatures above \(T_c\), we detect a spatially inhomogeneous magnetic field that tracks the hole-doping dependences of both \(T_c\) and the superfluid density at \(T = 0\) K. Our experiments are inconsistent with the field inhomogeneity above \(T_c\) being caused by electronic magnetic moments or a vortex liquid. Instead they are explained by the existence of nanometre-size superconducting regions with a local \(T_c\) that exceeds the bulk \(T_c\). In \(\text{YBa}_2\text{Cu}_3\text{O}_y\), we detect a spatially inhomogeneous response to field that persists beyond \(T = 200\) K, indicating that the basic ingredients for superconductivity near room temperature already exist in spatially localized regions of this material. A lingering question is the origin of the weak magnetism detected earlier in \(\text{YBa}_2\text{Cu}_3\text{O}_y\) by zero-field \(\mu\)SR, at temperatures below the pseudogap temperature \(T^*\).

This work was supported in part by the Swiss NSF under MaNeP and Division II.

10:24AM A2.00005 Observation of a Sharp Magnetic Transition at the Pseudogap Temperature in \(\text{YBa}_2\text{Cu}_3\text{O}_6\), HERB MOOK, Oak Ridge National Laboratory — Polarized neutron diffraction has been used to demonstrate magnetic order in a crystal of \(\text{YBa}_2\text{Cu}_3\text{O}_6\) that displays an exceptionally sharp superconducting transition. Earlier experiments showed a gradual increase of intensity of magnetically scattered neutrons from underdoped \(\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}\) crystals for reflections that do not break translational symmetry. The present experiment confirms this but displays a much sharper transition demonstrating that the width of the magnetic transition depends on the quality of the superconducting transition. This relationship is strengthened by the fact that other magnetic properties sensitive to the superconductivity, such the resonance and excitation spectra are also exceptionally well defined when measured with the same sample. The magnetic order is observed at the temperature of the pseudogap transition and the close relationship between the quality of the magnetic properties and the superconductivity suggests that the pseudogap is directly connected to the magnetic order.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A3 DCOMP TMS: Frontiers in Computational Materials

8:00AM A3.00001 Multi-Scale Modeling from First-Principles, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany and UC Santa Barbara, USA — Electronic structure theory (the nature of the chemical bond) is the base on which the finest scale for multi-scale modeling of the function of materials. Frequently it is assumed that details at this base do not matter when length and time scales approach meso- or macroscopic proportions (e.g. \(\mu\)m and minutes). In this talk I will show for various examples that details matter indeed. When accuracy is lacking at the base, there is little hope for predictive results at any level of modeling that follows. I will also emphasize the importance of reversible mapping and error control between the different levels of multi-scale modeling when moving up the chain of methods to successively increasing spatial and temporal dimensions. — In this context I will also address the sometimes problematic accuracy of present day density functional theory methods and show how it can be determined and errors corrected.

8:36AM A3.00002 Computational Approaches for Strongly Correlated Materials: an Electronic Structure Theory Perspective, SERGEY SAVRASOV, University of California Davis — Density functional theory known to work well for weakly correlated materials fails to attack real strongly correlated phenomena, and recent progress in understanding those using many-body model-hamiltonian-based dynamical mean-field theory has triggered developments of new approaches for computational material science in searching for alternatives to DFT. In this talk I will discuss some such new techniques, a spectral density functional theory, which considers total free energy as a functional of a local electronic Green function, will be discussed. Applications of the method to compute energetics, spectroscopy, lattice dynamics and exchange interactions of classes of materials such as heavy fermion and high temperature superconductors as well as actinide systems will be given.
9:12AM A3.00003 First-principles studies of electrical transport in nanoscale molecular junctions1. J. B. NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Understanding the conductance of individual molecular junctions is a forefront topic in theoretical nanoscience. The development of a general, efficient atomistic approach for treating an open system out of equilibrium with good accuracy, and then using it to inform experiment, is a significant open challenge in the field. Here I will describe studies where first-principles techniques, based on density functional theory (DFT) and beyond, are used to investigate some of the fundamental issues associated with single-molecule transport measurements. After a brief summary of previous work, a DFT-based scattering-state approach is presented and applied to H$_2$ and amine-Au linked molecular junctions [1], two systems for which there exist reliable data [2]. Similar to most ab initio studies, we rely on a Landaau approach within DFT for junction conductance. Using this framework, which has proven relatively accurate for metallic point contacts, good agreement with experiment is obtained for the H$_2$ conductance. For amine-Au linked junctions, however, the computed conductance is significantly larger than that measured, although structural trends are reproduced by the calculations. To explore this further, we draw on GW calculations of a prototypical metal-molecule contact, benzene on graphite, where interfacial polarization effects are found to drastically modify frontier orbital energies [3]. A physically motivated model self-energy correction is developed from our GW calculations, applied to the amine case, and shown to quantitatively explain the discrepancy with experiment. The importance of many-electron corrections beyond DFT for accurately computing molecular conductance and understanding experiments is thoroughly discussed. [1] S. Y. Quek et al., Nano Lett 7, 3482 (2007); K. H. Khoo et al., submitted (2007). [2] R. Smit et al., Nature 419, 906 (2002); L. Venkataraman et al., Nature 442, 904 (2006). [3] J. B. Neaton et al., Phys. Rev. Lett. 97, 216405 (2006).

1This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

9:48AM A3.00004 First-Principles Thermodynamics and Kinetics of Advanced Hydrogen Storage Materials1. VIDVUDS OZOLINS, Department of Materials Science & Engineering, University of California, Los Angeles — Hydrogen-fueled vehicles require a cost-effective, light-weight material that binds hydrogen strongly enough to be stable at ambient pressures and temperatures but weakly enough to liberate H$_2$ with minimal heat input. Since none of the simple metal hydrides satisfy all the requirements for a practical H$_2$ storage system, recent research efforts have turned to complex hydrides and advanced multicomponent material compositions. We will show that first-principles density-functional theory (DFT) calculations have become a valuable tool for understanding and predicting novel hydrogen storage materials. Recent studies in our group have used DFT calculations to (i) predict crystal structures of new solid-state hydrides, (ii) determine phase diagrams and thermodynamically favored reaction pathways in multinary hydrides, and (iii) study microscopic kinetics of diffusion, phase transformations, and hydrogen release.

1Research supported by US DOE grants DE-FG02-05ER46253, DE-FG02-07ER46433, and by NSF grant CBET-0730044.

10:24AM A3.00005 Liquid Metal Embrittlement: new understanding for an old problem. DAVID SROLOVITZ, Yeshiva University — When liquid metals are brought into contact with other polycrystalline metals, deep liquid-filled grooves often form at the intersections of grain boundaries and the solid-liquid interface. In some systems, e.g., Al-Ga, Cu-Bi and Ni-Bi, the liquid film quickly penetrates deep into the solid along the grain boundaries and leads to brittle, intergranular fracture under the influence of modest stresses. This is a form of liquid metal embrittlement (LME). This phenomenon is ubiquitous in material processing and is particularly important in nuclear reactor scenarios in which liquid metals are used as coolants and as spallation targets. The penetration of a liquid phase along the grain boundary is a complex phenomenon, involving several different types of simultaneous processes. The tendency for and rate of LME are also sensitive to externally controllable factors such as temperature and applied stress. Because of the interplay between the underlying phenomena that occur in LME, it has been difficult to perform experiments that can be interpreted to understand which processes control LME and which are simply parasitic. We study LME by performing molecular dynamics simulations of an Al bicrystal in contact with liquid Ga and investigate how Ga penetrates along the grain boundaries during the early stages of the wetting process. We use the simulation results to propose a new mechanism for LME and compare it with general trends gleaned from a series of LME experimental studies.

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A4 DPOLY: Polymers at Surfaces: Adhesion, Tribology and Patterning Morial Convention Center 206

8:00AM A4.00001 Interfacial engineering using heteropolymers with adjustable monomer sequences (HAMS)1. JAN GENZER, Department of Chemical & Biomolecular Engineering, North Carolina State University — Heteropolymers with adjustable monomer sequences (HAMS) represent a new type of functional random copolymers that could play an important role in emerging areas pertaining to interfacial science and polymer assembly. Due to their disordered but tailorable co-monomer sequence distribution HAMS are capable of adsorbing selectively at interfaces and recognizing patterns on chemical targets (i.e., chemically patterned substrates). HAMS are synthesized in a laboratory by ‘coloring’ the segments of a collapsed homopolymer, A, with a functionalizing agent, B, and then unraveling the resultant polymer to yield a random sequence of A and B blocks, which ‘remembers’ its original collapsed conformation and hence prefers some conformations over others. In the presentation, we will provide details pertaining to the experimental formation of HAMS and studying their physico-chemical characteristics. We will also provide examples of a few case studies that unravel the tailorable interfacial and self-assembly character of HAMS made of poly(styrene-co-4-bromostyrene) and its derivatives. In addition, we present results of computer simulation studies providing molecular insight into forming HAMS.

1Supported by the NSF-DMR Polymers Program.

8:36AM A4.00002 Carbon Nanotube-Based Synthetic Gecko Tapes, ALI DHINOJWALA, The University of Akron — Wall-climbing geckos have unique ability to attach to different surfaces without the use of any viscoelastic glues. On coming in contact with any surface, the micron-size gecko foot-hairs deform, enabling molecular contact over large areas, thus translating weak van der Waals (vdW) interactions into enormous shear forces. We will present our recent results on the development of synthetic gecko tape using aligned carbon nanotubes to mimic the keratin hairs found on gecko feet. The patterned carbon nanotube-based gecko tape can support a shear stress (35 N/cm$^2$) nearly four times higher than the gecko foot and stick to a variety of surfaces, including Teflon. Both the micron-size setae (replicated by nanotube bundles) and nanometer-size spatulas (individual nanotubes) are necessary to achieve macroscopic shear adhesion and to translate the weak vdW interactions into high shear forces. The carbon nanotube based tape offers an excellent synthetic option as a dry conductive reversible adhesive in microelectronics, robotics and space applications. The mechanism behind these large shear forces and self-cleaning properties of these carbon nanotube based synthetic gecko tapes will be discussed. This work was performed in collaboration with graduate students Liehui Ge, and Sunny Sethi, and collaborators from RPI, Lijie Ci and Professor Pulickel Ajayan.
9:12AM A4.00003 Polymer adhesion at surfaces: biological adhesive proteins and their synthetic mimics¹. PHILLIP MESSERSMITH, Northwestern University — Mussels are famous for their ability to permanently adhere to a wide variety of wet surfaces, such as rocks, metal and polymer ship hulls, and wood structures. They accomplish this through specialized proteins collectively referred to as mussel adhesive proteins (MAPs). The biophysical aspects of MAP adhesion is being revealed through the use of single molecule force measurements. The results provide insight into the adhesive roles of key amino acids found in these proteins, including the magnitude of adhesive forces, cooperative effects, and their self-healing properties. This molecular-level information is being incorporated into designs of biomimetic polymer coatings for a variety of applications. Our biomimetic approach to polymer design will be illustrated by a few examples where adhesive constituents found in MAPs are exploited to make wet-adhesive polymer coatings. In addition, small molecule analogs of MAPs can be used to apply thin functional films onto virtually any material surface using a facile approach. These coatings have a variety of potential uses in microelectronics, water treatment, prevention of environmental biofouling, and for control of biointerfacial phenomena at the surfaces of medical/diagnostic devices.

¹Research supported by NIH grant DE014193.

9:48AM A4.00004 Patterning inorganic nanoparticles in Polymer Films. EUGENIA KUMACHEVA, University of Toronto — No abstract available.

10:24AM A4.00005 Wrinkling, Crumpling and Snapping for Surface Property Control, ALFRED CROSBY, University of Massachusetts Amherst — Upon the development of a critical stress, many materials and geometries experience a mechanical instability, which produces significant changes in geometry with very small changes in stress. In nature, mechanical instabilities are ubiquitous with the definition of shape, morphology, and function. Examples range from wrinkles on human skin to the snapping of Venus Flytrap leaflets. Inspired by these examples and others, we use elastic instabilities to control the morphology and function of soft polymer surfaces. We present three strategies. The first is a novel approach for the development of surface wrinkles on a top-constrained elastomer surface. We demonstrate and understand the control of kinetically-trapped and equilibrium wrinkle morphologies associated with changes in the materials properties and geometric constraint. These structures are stabilized to create surfaces with enhanced adhesion and advantageous optical properties. A second strategy is based on the controlled buckling of surface attached sheets. This method allows the fabrication of responsive surface structures that are prone to snap-through instabilities and the fabrication of pattern features that are difficult, if not impossible, to achieve with any other method. The third strategy brings the bio-inspired surface control full circle with the use of mechanical instabilities to control and characterize monolayer sheets of biological cells.

Monday, March 10, 2008 8:00AM - 11:00AM
Session A5 DCMP: Supersolid 4He: A New State of Matter Morial Convention Center RO1

8:00AM A5.00001 Probable heat capacity signature of the supersolid transition¹. XI LIN, Penn State University — We report our heat capacity measurements [1] of solid ⁴He down to 40mK, well into the apparent supersolid region of the phase diagram. We observed a broad peak in the specific heat centered near 75mK in ⁴He samples containing 1ppb, 0.3ppm, and 10ppm ³He impurities. In addition, our measurements of samples containing 10ppm and 30ppm of ³He have revealed a temperature-independent contribution to the heat capacity that scales with the number of isotopic impurities. New measurements with higher resolution are in progress.


¹Experiment carried out in collaboration with A. C. Clark and M. H. W. Chan with support from NSF under grants DMR-0207071 and DMR-0706339.

8:36AM A5.00002 Probing the upper limit of the nonclassical rotational inertia². ANN SOPHIE C. RITTNER, Cornell University — Recently, we have used torsional oscillators to study the dependence of the nonclassical rotational inertia on sample confinement, expressed as surface to volume ratio S/V [1]. When we decreased the width of annular helium sample we observed an increase of the supersolid fraction by three orders of magnitude to 20 % in a 150 µm wide annulus. As an extension of those measurements, we have built torsional oscillators with even smaller gaps down to 25 microns. We will give a brief description of the experimental setup and present the results of those measurements.


²Work supported by NSF Grant DMR-0605864

9:12AM A5.00003 Frequency dependence and Hysteretic behavior in Non-Classical Rotational Inertia of Solid ⁴He³. YUKI AOKI², Rutgers University — We have constructed a compound torsional oscillator having two resonance frequencies for studying non-classical rotational inertia (NCRI) of solid ⁴He. The oscillator allows us to study NCRI and supersolid effects of the identical solid ⁴He sample grown in a cylindrical container at 496 and 1173 Hz. We have grown and studied solid samples with final solid pressures between 27 and 42 bar. The observed features are qualitatively similar in all solid samples. NCRI fractions at sufficiently low oscillation drive and at the lowest temperature are only about 0.1 % and consistent with cylindrical cells in other laboratories. NCRI fraction below 35 mK does not depend on frequency nor temperature. At T > 35 mK, NCRI fraction observed in the lower mode is smaller than that in the higher mode. “Transition” into supersolid state occurs at a higher temperature in the higher mode than the lower one. The peak in extra dissipation due to solid ⁴He is greater in the lower mode by a factor 1.7 than in the higher mode. The frequency dependence of the magnitude of NCRI will be compared with existing theoretical predictions. In addition to the frequency dependent effects at low oscillation drive, we have observed hysteretic behavior in NCRI fraction depending on the history of oscillation drive and temperature from the normal state above 300 mK to low temperatures. We find that the supersolid state below 40 mK can have different NCRI fractions depending on the particular sequence of oscillation amplitude. Above about 50 mK, however, NCRI fraction does not depend on the history of oscillation amplitude changes. We also observe a time dependent overshoot in the dissipation of solid when the NCRI fraction is increased by decreasing the oscillation drive. The general behavior of this relaxation phenomenon is rather complex depending on temperature, history of oscillation amplitude and memory effects. Some of the observations share common features with vortex motion and glassy behavior.

³Research supported by NSF DMR0704120.

²In collaboration with Michael C. Keiderling, Joseph C. Graves and Harry Kojima.
9:48AM A5.00004 Superfluid defects in solid Helium-4: grain boundaries, dislocations, superglass\textsuperscript{1}. NIKOLAY PROKOF'EV, University of Massachusetts, Amherst, MA 01003, USA — First principle quantum Monte Carlo simulations and recent experiments all point out that ideal, defect free, crystals of Helium-4 are not supersolid. Contrary to naive expectation that disorder inhibits superfluidity and suppresses superfluid response due to localization effects, disorder in quantum solids works in the opposite direction: if particles in the ideal crystal are already localized then defects can help to make the sample superfluid. The theory of superfluidity in lower dimensional defective structures embedded in a higher dimensional bulk has its own twists since such phenomena as superfluidity, roughening and defect mobility may be strongly linked. An unusual behavior is expected in the 3D network of 1D liquid channels when normal state at temperatures orders of magnitude above T\textsubscript{c} is indistinguishable from that of a superfluid. The possibilities for “designing” crystallographic defects are countless, and in the strongly correlated system each case (superfluid or not) has to be considered separately. We find that generic grain boundaries and the screw dislocation along the z-axis are superfluid, while special types of boundaries and edge dislocations are insulating [1,2]. We also find that Helium-4 can form a metastable superfluid glass [3]. Whether these findings are relevant for the explanation of supersolid and other experiments remains an open question.


NSF support

10:24AM A5.00005 Vortex liquid, PHILIP ANDERSON, Princeton University — No abstract available.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A6 FIAP: Novel Channel Materials for CMOS Technology Morial Convention Center R04

8:00AM A6.00001 III-V MOSFETs: From Materials & Physics to Devices, MATTHIAS PASSLACK, Freescale Semiconductor, Inc. — Gallium-Arsenide metal-oxide-semiconductor field-effect-transistors (MOSFET) have finally been demonstrated with performance metrics matching the predictions of semiconductor device models. Recent discoveries and inventions in many areas including materials and fabrication, semiconductor physics, interface chemistry, semiconductor interface analysis, and semiconductor device design and process have contributed to this success. In my invited talk, I will review some areas including the unique properties of interfaces formed between Ga\textsubscript{2}O\textsubscript{3} molecules and a GaAs surface, a high permittivity (\textit{\varepsilon} \geq 20) Ga\textsubscript{2}O\textsubscript{3}/Ga\textsubscript{2}O\textsubscript{3} dielectric stack providing both a device quality interface and band-offsets on GaAs required for MOSFET operation, a semiconductor heterostructure for mitigation of high band-edge interface-state density, and device design criteria for high electron channel mobility and MOSFET drive current. Performance metrics of present metal-gate GaAs enhancement-mode MOSFETs such as electron channel mobility, drive current, transconductance, and threshold voltage will be discussed. GaAs MOSFETs with In\textsubscript{0.35}Ga\textsubscript{0.65}As channel layers exhibit typical electron peak mobilities exceeding 5,000 cm\textsuperscript{2}/Vs, an improvement of a factor of 20 over silicon based high-\textit{\varepsilon} metal-gate inversion-mode MOSFETs. Even higher electron mobilities surpassing 12,000 cm\textsuperscript{2}/Vs have been measured in In\textsubscript{0.75}Ga\textsubscript{0.25}As channel layers. Beside the use of channel materials such as In\textsubscript{x}Ga\textsubscript{1-x}As with high bulk electron mobility, the physics of device operation is distinctively different from silicon inversion-mode MOSFETs. III-V MOSFET are now considered an option for CMOS based circuitry beyond the 22 nm node of the International Technology Roadmap for Semiconductors. High channel mobilities and the first successful implantation of III-V MOSFETs seem to justify such contemplation, however, many obstacles remain.

8:36AM A6.00002 Stability of Metal Oxide/Ga and Metal Oxide/III-V Interfaces and Implications for Low Defect Density MOS Devices\textsuperscript{1}, PAUL MCINTYRE, Stanford University — The need to achieve high performance in MOS transistors as they scale to their ultimate size limits prompts interest in channel materials, such as Ge and III-V compound semiconductors, which exhibit larger intrinsic carrier mobilities than Si. Given the need to reduce gate leakage current density while maintaining electrostatic control of the devices, it is necessary to deposit high-\textit{\varepsilon} gate dielectrics onto these novel channel materials. Unlike silicon, high mobility channel materials do not form a highly-stable and stoichiometric native oxide; therefore, control of the state of oxidation at the metal oxide dielectric/channel interface during and after gate dielectric deposition is essential. This presentation will summarize findings reported to date on 1) chemical stability of Ge and III-V surfaces in the presence of oxygen and 2) oxide/channel defect formation and passivation. New results on pre-high-\textit{\varepsilon} chemical surface preparation, structural modification during metal oxide deposition and the resulting effects on MOS capacitor and transistor characteristics will also be presented, with emphasis on Al\textsubscript{2}O\textsubscript{3} and HFO\textsubscript{2} gate insulators grown by atomic layer deposition onto Ge and InGaAs channels. In situ and ex situ monitoring of chemical bonding at the gate insulator/channel interface by photoelectron spectroscopy will be correlated with the D\textsubscript{ltf}, fixed charge and charge trapping behavior of MOS devices.

\textsuperscript{1}Financial support from the SRC Nonclassical CMOS Center and from Intel Corporation is gratefully acknowledged.

9:12AM A6.00003 Dangling-bond defects and hydrogen passivation in germanium, JUSTIN R. WEBER, Department of Physics, University of California, Santa Barbara, California 93106-9530, USA — The application of germanium in complementary metal-oxide semiconductor (CMOS) technology is hampered by high interface-state densities, the microscopic origin of which has remained elusive. Using first-principles calculations, we have investigated the atomic and electronic structure of prototype germanium dangling-bond defects [1]. The computational approach is based on density functional theory, and in order to overcome band-gap problems we have also performed quasiparticle calculations based on the GW approach. Surprisingly, the germanium dangling bonds give rise to electronic levels below the valence-band maximum. They therefore occur exclusively in the negative charge state, explaining why they have eluded observation with electron spin resonance. The associated fixed charge is likely responsible for threshold-voltage shifts and poor performance of n-channel transistors. At silicon/silicon dioxide interfaces, hydrogen is successfully used to passivate dangling-bond defects. We have therefore also investigated the interaction of hydrogen with germanium. In contrast to silicon and other semiconductors in which hydrogen behaves as an amphoteric impurity, interstitial hydrogen in germanium is stable only in the negative charge state, i.e., it behaves exclusively as an acceptor. Passivation of dangling bonds by hydrogen will therefore be ineffective, again explaining experimental observations. Other cases where unusual interfacial defects and problems with hydrogen passivation may occur will be discussed.

Work performed in collaboration with A. Janotti, P. Rinke, and C. G. Van de Walle, and supported by the Semiconductor Research Corporation.

9:48AM A6.00004 Scanning-tunneling microscopy and spectroscopy of oxide deposition on III-V semiconductor surfaces, ANDREW KUMMEL, UCSD — The correlation between the atomic bonding structure and the electronic structure at oxide-semiconductor interfaces is critical to understanding how atomic scale changes in electronic structure can cause localization of electrons or holes at these interfaces. All logic devices function by having an electric field perturb the electronic structure of a semiconductor to change its resistance thereby activating the device. The key material in this process is the interface between the gate oxide and the semiconductor. Any fixed charge or defects which trap electrons or holes destroy the device operation because the electric field will be terminated by interface charges instead of being transmitted into the semiconductor. We have used atomically resolved scanning tunneling microscopy (STM) imaging and current-voltage (I-V) tunneling spectra (STS) to determine the atomic and electronic structure at the gate-oxide semiconductor interface. Our research focuses upon the group III-V semiconductors (GaAs, InGaAs, InAs) since they offer electron speeds up to 30x greater than silicon as well as germanium since it offers 3x higher hole speeds than silicon. In general, electronically passive interface forms are encountered when oxide deposition does not disrupt the semiconductor lattice but instead restores the semiconductor surface atoms back to more bulk-like electronic structure. Even in the absence of a lattice disruption, oxide deposition can create new states in the bandgap thereby pinning the Fermi level by two mechanisms: direct (the adsorbate induced states in the bandgap region) and/or indirect (generation of undimerized surface atoms).


Monday, March 10, 2008 8:00AM - 11:00AM — Session A7 DBP GSNP: Oscillations Without Transcription in Vivo and in Vitro Morial Convention Center R05

8:00AM A7.00001 Molecular synchronization, the Kai system, and biological oscillators, DAVID K. LUBENSKY, University of Michigan — In most textbook examples, oscillations in cell biology are driven by the periodic creation and destruction of one or more chemical species. The past few years, however, have seen growing interest in a different sort of oscillator. In these systems, the total concentrations of the major protein components are constant, but the molecules move sequentially through a cycle of different states (e.g., covalent modifications). Macroscopic oscillations appear when the progress of the many individual molecules becomes synchronized. The recently-characterized cyanobacterial circadian clock provides a particularly elegant example of such molecular synchronization. Remarkably, with only the 3 proteins KaiA, KaiB, and KaiC, a ~24 hour oscillation in KaiC phosphorylation can be reconstituted in vitro. We can thus dissect this biochemical circuit in almost unprecedented detail. Here, we give an overview of the Kai system and its relationship to other oscillators. We begin with a review of the major experimental facts about the Kai system, emphasizing possible mechanisms to synchronize KaiC phosphorylation. We then examine in more detail models in which this synchronization occurs through sequestration of KaiA via differential affinity: KaiA, which stimulates KaiC phosphorylation, has a higher affinity for KaiC during certain stages of the phosphorylation cycle; as long as some KaiC molecules at these stages are present in the reaction mixture, they bind all the available KaiA, thereby preventing the other KaiC’s from being phosphorylated and proceeding through the cycle. We also discuss the implications of this mechanism for phenomena such as temperature compensation. Finally, we suggest that, in light of lessons learned from the Kai system, a number of other biological oscillators can fruitfully be viewed as examples of molecular synchronization.

8:36AM A7.00002 Monomer exchange and the hourglass model of protein-based oscillators, ELDON EMBERLY, Physics, Simon Fraser University — Circadian rhythms in photosynthetic cyanobacteria are under the control of a three protein biochemical network that generates oscillations in the phosphorylation level of one of the proteins. This oscillatory signal has a period of roughly 24 hours and regulates many biological processes in the bacteria to the day and night cycle. The molecular view of the phosphorylation process is that one of the proteins forms a hexameric complex whose phosphorylation levels rise and fall based on the activity of the other two proteins. Each hexameric complex thus functions as an independent molecular clock. However the bacteria contains many such clocks and so how do they interact to generate a coherent oscillating signal? In this talk I will discuss a model that suggests that monomer exchange between hexamers helps to synchronize the population of clocks during the daylight portion of the oscillation. Other synchronizing mechanisms will be highlighted for the other portion of the cycle. Recent experiments will be discussed in light of the exchange model.

9:12AM A7.00003 Perfect Robust Network Architecture of a Bacterial Circadian Clock, MARKUS KOLLMANN, Humboldt Universität zu Berlin, Invalidenstr. 43, 10115 Berlin — The circadian core clock of cyanobacteria consists of only three proteins, KaiA, KaiB, and KaiC. The readout of the clock status is given by the phosphorylation level of KaiC hexamers that oscillates with 23 hour period even under in vitro conditions. We present a circadian clock model based on mass action kinetics that shows almost perfect agreement with the experimentally found phosphorylation dynamics. The model consists of two feedback loops, with the main oscillatory mechanism realised by a negative feedback via sequestration of the enhancer of KaiC autophosphorylation, that is KaiA. These feedbacks are the reason for the observed outstanding robustness of the KaiABC clock that keeps phase, frequency and amplitude even under concerted serveral fold changes of the Kai protein concentrations.

9:48AM A7.00004 Stability and Noise in the Cyanobacterial Circadian Clock, IRINA MIHALCESCU, Université Joseph Fourier — Grenoble — Accuracy in cellular function has to be achieved despite random fluctuations (noise) in the concentrations of different molecular constituents inside and outside the cell. Single cell in vivo monitoring reveals that individual cells generate autonomous circadian rhythms in protein abundance. In multi-cellular organisms, the individual cell rhythms appear to be noisy with drifting phases and frequencies. However, the whole organism is significantly more accurate, the temporal precision being achieved most probably via intercellular coupling of the individual noisy oscillators. In cyanobacteria, we have shown that single cell oscillators are impressively stable and a first estimation rules out strong intercellular coupling. Interestingly, these prokaryotes also have the simplest molecular mechanism at the heart of their circadian clock. In the absence of transcriptional activity in vivo, as well alone in vitro, the three clock proteins KaiA, KaiB and KaiC generate a self-sustained circadian oscillation of autophosphorylation and dephosphorylation. Recent chemical kinetics models provide a possible understanding of the three-protein oscillator, but the measured in vivo stability remains yet unexplained. Is the clock stability a built-in property of the cyanobacterial clock mechanism? Recent experiments will be discussed in light of the diffusion constant. These results therefore confirm that the cyanobacterial clock stability is a built-in property: the cyanobacterian clock mechanism is not only the simplest but also the most robust.
10:24AM A7.00005 Chromosome oscillations in mitosis. OTGER CAMPAS, Harvard University — Successful cell division necessitates a tight regulation of chromosome movement via the activity of molecular motors. Many of the key players at the origin of the forces generating the motion have been identified, but their spatial and temporal organization remains elusive. In animal cells, chromosomes periodically switch between phases of movement towards and away from the pole. This characteristic oscillatory behaviour cannot be explained by the current models of chromosome positioning and congression. We perform a self-contained theoretical analysis in which the motion of the kinetochore and chromokinesins results from the competition between the activity of the kinetochore and chromokinesins motors on the chromosome arm. Our analysis, consistent with the available experimental data, proposes that the interplay between the aster-like morphology of the spindle and the collective kinetics of molecular motors is at the origin of chromosome oscillations, positioning and congression. It provides a natural explanation for the so-called chromosome directional instability and for the mechanisms by which chromosomes sense their position in space. In addition, we estimate the in vivo velocity of chromokinesins at vanishing load and propose new experiments to assess the mechanism at the origin of chromosome movement in cell division.

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A8 DFD: Colloidal Self-Assembly | Morial Convention Center R06

8:00AM A8.00001 Directed Self-Assembly of Spherical Particles , NATALIE ARKUS, GUANGNAN MENG, VINOTHAN MANOHARAN, MICHAEL BRENNER, Harvard University — We examine the kinetics and energetics of self-assembly in systems containing a small number of spherical colloidal nanoparticles using a combination of theory, simulation, and experiment. We then explore how the addition of spherically symmetric binding specificity can be used to direct the self-assembly of a given structure. Using graph theoretic, numerical, and algebraic geometric techniques, we enumerate all possible packings for a system of n particles. We map out the energetic landscape of these packings, which is determined not only by the value of the potential energy at these minima, but also by the vibrational normal modes of the structures. Experiments for a 6 particle system show that the likelihood of a given packing follows this expected equilibrium distribution. To explore the kinetics of packing formation, we simulate the self-assembly of these systems in the irreversible binding limit. For the 6 particle system, this reveals that the kinetics required to form one of the packings is highly unlikely, resulting in the other packing forming with 100% probability. With the addition of binding specificity however, we can cause the unlikely packing to form with 100% probability. We show how the addition of binding specificity effects the energetic landscape of these systems, and that it alone is sufficient to direct self-assembly.

8:12AM A8.00002 Controlling assembly of micro- and nano-particle systems with DNA. , DMYTRO NYKYPANCHUK, MATHEW MAYE, DANIEL VAN DER LELIE, OLEG GANG, Brookhaven National Laboratory — Addressable biological interactions provide attractive platform for rational self-assembly, however the strength of such interactions are often difficult to control. Here we present an approach where DNA molecules are used to balance attractive and repulsive interactions during particle assembly while preserving the interaction addressability. We show, that by changing the composition and structure of DNA shall of micro- (2 um) or nanoparticles (10 nm), assembly kinetics, aggregate sizes, and the systems melting properties can be tuned. At constant environmental conditions, this strategy allows for rational control of interaction energy landscape for nano- and micro-systems in a wide dynamic range.

8:24AM A8.00003 Evaporation-Driven Assembly of Microspheres with Polymer in Emulsion Droplets1, KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan, LIANG-JIE LAI, Dept. of Physics, National Central University, Chung-li, Taiwan, CHIH-CHUNG CHANG, HUI CHEN, Dept. of Chemical and Materials Engineering, National Central University, Chung-li, Taiwan — We study the packing of colloidal microspheres mixed with polymer in oil-in-water emulsion droplets through evaporation. The addition of polymer produce non-unique configurations of final clusters when the number of particles N inside the droplet is larger than 4. The cluster configurations are classified into three categories based on the symmetry. Stabilized colloidal clusters of spherical packings are observed. Observation on packing process shed light to the mechanisms which cause different and non-unique structures. The osmotic pressure and interparticle interaction due to polymer play important roles in packing.

1Support for this work is provided by NSC Grant No. 96-2112-M-001

8:36AM A8.00004 Entropy-driven self-assembly of dimers , ISSEI NAKAMURA, AN-CHANG SHI, McMaster University — Supramolecular self-assembly is an important phenomenon with applications ranging from chemical synthesis to biological systems. Although the driving force of assembly is the weak non-covalent intermolecular interaction such as hydrogen bonding and dispersion force, the self-assembly is a result from balancing the enthalpic and entropic contributions. In general, the disassembled/disordered phase is expected as temperature is raised because of the entropic gain from the components of the aggregate. However, it has been observed that the self-assembled/ordered phase can be promoted with increasing temperature. This implies that the self-assembly is driven by entropy. In order to provide a better understanding of this entropy-driven transition, we have studied a statistical mechanical model for the aggregation of macromolecular dimers immersed in solvents. The model demonstrates that solvent molecules absorbed on the surface of the solution are released with increasing temperature, leading to an increase of the total entropy of the system. Consequently, the cooperative stability of the dimeric state is induced. The thermodynamic features of this transition are analyzed.

8:48AM A8.00005 Hydrodynamic interactions effects on the dipole-induced self-assembly of β-peptides and Brownian-induced polymer pore translocation , JUAN HERNANDEZ-ORTIZ, Departamento de Materiales, Universidad Nacional de Colombia, Sede Medellín, MICHAEL GRAHAM, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — A novel method that scales linearly with the number of particles is used to study Brownian-systems considering fluctuating hydrodynamic interactions. The method is demonstrated in the concept of two applications: the dipole-induced self-assembly of β-peptides and the Brownian-motion-induced translocation of a polymer thought a rectangular pore. The method includes the long-range interactions by the Green’s function formalism. It allows the consideration of peptides at intermediate concentrations and the inclusion of the non-periodic domain of the translocation. The hydrodynamics interactions affect the dynamics of the peptides agglomeration and the mean-square-displacement indicates significant changes in the long-time diffusion coefficient. The polymer translocation is study using a transition path sampling based methodology. In particular it is used to calculate the translocation rate constant. Even for a single bead there are differences once hydrodynamics are included. These differences are due to the changes of mobility near walls and the change in polymer chain diffusion coefficient.

9:00AM A8.00006 Self-assembly of complex shaped colloidal particles , ADELINA PERRO, VINOTHAN N. MANOHARAN, Harvard School of Engineering and Applied Sciences — We have developed a new method to produce hybrid particles with polyhedral shapes in very high yield (liter quantities at up to 75% purity) using a combination of emulsion polymerization and inorganic surface chemistry. The optical properties of these particles are tailored for studying their dynamics and self-assembly. For example, we produce systems that consist of index-matched sphere doublets with a small strongly scattering inorganic core between the two spheres, allowing us to track the center of mass of each doublet. We have generalized the preparation procedure to create even more complex geometries, including hybrid tetrahedra and octahedra. We present some preliminary studies on the self-assembly of these systems based on various optical experiments, including confocal microscopy, light scattering, and digital holographic microscopy.
9:12AM A8.00007 Progress on systems of DNA modified colloidal particles for self-replication, PAUL CHAIKIN, MIRIAM LEUNISSEN, REMI DREYFUSS, ROUJIE SHA, NADRIAN SEEMAN, DAVID GRIER, DAVID PINE, New York University — Our goal is to create new materials that can self-replicate and self-assemble. For this, we modify the interactions between micrometer-sized colloids by coating them with single-stranded DNA ‘sticky ends’, which specifically recognize complementary sequences on other colloids. We find that the aggregation-dissociation behavior is fully reversible for at least tens of temperature cycles. Using magnetic beads or optical tweezers, we form a chain-like ‘seed’ structure, which acts as a template to assemble colloids. The system is collimated by a high degree of orientational organization. Factors that determine the crystal structure are investigated, especially the dependence on ionic strength and on Janus balance. Contrary to the transverse linkers, the longitudinal linkers form AT/TA bonds, which can be crosslinked with an intercalator and UV irradiation. In this way, we permanently fix the seed and its copies.

9:24AM A8.00008 Binary Colloidal Assembly by Dielectrophoresis, PETER HOFFMAN, YINGXI ELAINE ZHU, University of Notre Dame — Dielectrophoresis (DEP)-driven colloidal assembly has been recently explored as a new route to manipulate colloids and rapidly form nanostructured materials. In this talk, we demonstrate that colloidal particles of varied sizes can be assembled with controllable packing configurations in the presence of AC-electrical fields. We investigate binary latex particles of varied size ratios from 0.25 to 0.8 and directly monitor the dynamic assembly process with final structural characterization by using high-speed confocal microscopy. We observe rich phase behaviors of binary colloidal assembly with a strong dependence of applied AC-field frequency and medium conductivity. The obtained structural phase diagram can be well predicted by the DEP mobility and the Peclet number. We also present a mechanism that underlies the colloidal charge polarization due to charge segregation and entrainment within the double layer at several distinct frequencies, which cannot be explained by the classical Maxwell-Wagner theory. We recently also employ the same mechanism to form binary colloidal crystals.

9:36AM A8.00009 Unusual aggregation behavior of colloids coated with palindromic DNA, MIRIAM LEUNISSEN, REMI DREYFUSS, DAVID PINE, PAUL CHAIKIN, New York University — Coating particles with single-stranded DNA ‘sticky ends’ gives excellent control over the specificity, strength and range of their interactions. Usually, a pair of complementary ‘Watson-Crick’ sequences is used to obtain thermoreversible binding of different colloids. However, for certain purposes one could also use self-complementary ‘palindrome’ sequences. Using light microscopy, we studied the aggregation behavior of micrometer-sized palindromic-coated colloids. Unlike Watson-Crick sticky ends, we found that it is of great importance whether the palindrome sticky end is attached to a flexible single strand or a rigid double-stranded ‘rod’. While the latter system displayed normal dissociation at elevated temperature, the former system showed enhanced aggregation with increasing temperature and no aggregation during fast temperature quenches. We explain these unusual observations by a competition between intra- and interparticle bonds. This provides us with an additional level of control over the interparticle bonding, besides the sequence of the sticky ends, the salt concentration and the DNA density on the beads.

9:48AM A8.00010 Functionalized Au nanoparticles in solution, GARY S. GREST, J. MATTHEW D. LANE, Sandia National Labs — The properties of functionalized Au nanoparticles in decane and water were studied by large-scale explicit atom, molecular dynamics simulations. Gold nanoparticles functionalized with S-(CH$_2$)$_n$-X alkanethiol chains (X = COOH or CH$_3$) were studied at the liquid-vapor interface and in the bulk. The structure of the functional groups on the nanoparticle was found to depend strongly on the end group and solvent. At the interface methyl terminated nanoparticles repel the water and move toward the vapor while in decane, the decane molecules engulf the nanoparticle. In the bulk, results for the nanoparticle/ nanoparticle pair correlation function and nanoparticle diffusion will be presented as a function of nanoparticle concentration. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04- 94AL85000.

10:00AM A8.00011 DNA-Grafted Janus Particles, CHING HSUEH, Department of Physics, National Central University, Chungli, Taiwan, KENG-HUI LIN, WEN-TAU JUAN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Recently there have been advances in generating Janus microspheres whose two hemispheres have different chemical compositions [1-4]. The new types of particles open up possibilities for assembly of complex structures. Here we attach DNA molecules onto one side of Janus microspheres. The new type of colloidal particles resembles surfactant molecules and may provide us interesting new structures.


10:12AM A8.00012 The importance of repulsion in the aggregation-dissociation behavior of DNA coated colloids, REMI DREYFUSS, MIRIAM LEUNISSEN, ROUJIE SHA, NADRIAN SEEMAN, DAVID GRIER, DAVID PINE, PAUL CHAIKIN, New York University — Coating particles with DNA gives excellent control over the specificity, strength and range of their interactions. In our experiments, a pair of complementary ‘Watson-Crick’ sequences is used to obtain thermoreversible binding of different colloids. Colloids coated with such complementary ‘sticky’ DNA aggregate when they are mixed together, the aggregates dissolve again when they are heated. We investigate the melting behavior of colloids coated with both sticky and non-sticky DNA. By changing the ratio between the sticky and non-sticky DNA, the obtained melting curves have very different melting temperatures, but almost the same sharpness. We show that the sharpness does not change because a high number of bonds bridges the particles, and that the strong shift in melting temperature is due to a repulsive interaction induced by the confinement of the non-sticky DNA when the particles come close together.

10:24AM A8.00013 Self Assembly of Colloidal Particles at Small N, GUANGNAN MENG, NATALIE ARKUS, RYAN MCGORTY, MICHAEL BRENNER, VINOTHAN MANOHARAN, Harvard University — We confine a small number (N ≈ 10) of micron-sized colloidal particles within micro-wells, and we use this finite system to study the process of self-assembly. The reversible aggregation of colloidal particles is controlled by a short-range depletion attraction, which is induced by poly(N-isopropylacrylamide) nano particles. We use digital holographic microscopy to monitor the structural and kinetic properties of self-assembled colloidal clusters, and we use micro-wells to collect ensemble statistics. We compare our experimental results with theory and simulations, which probe how energetics and kinetics affect the packing structures.

10:36AM A8.00014 2D crystals of Janus amphiphilic colloidal spheres, SHAN JIANG, STEPHEN ANTHONY, University of Illinois at Urbana-Champaign, ANGELO CACCIUTO, Columbia University, ERIK LUIJKEN, STEVE GRANICK, University of Illinois at Urbana-Champaign — Colloidal spheres with one side hydrophilic and the other side hydrophobic form 2D crystals with hexagonal translational order complemented by a high degree of orientational organization. Factors that determine the crystal structure are investigated, especially the dependence on ionic strength and on Janus balance. Depending on these variables, patches of the orientational order can be altered: from doublets to extended lines containing dozens of particles. Janus particles with different geometry (Janus balance) self-assemble into different cluster structures. Collective motion is evident from time-resolved optical microscopy.
which point the efficiency is also predicted to reach a maximum. Operating range, and show excellent agreement with the experiments. The propulsive force is predicted to increase sharply after the shape transformation, at is complete. Calculations based on slender body and resistive force theory predict the torque-speed relationship and the filament shape throughout the entire by a sharp increase in the rotational speed. As the torque is decreased, the shape change exhibits hysteresis, transitioning back to the splayed form at a lower . rod rotating in a viscous fluid and set at an angle to the axis of rotation. In the experiments, two modes of operation are studied: constant torque and constant .

E. coli in a viscous fluid

Lagrangian methods in combination with the Maxey-Riley equations for inertial particles in fluid flow.

used to illustrate the proposed approach. We also show that predator-prey interactions during jellyfish swimming can be addressed using the aforementioned underwater velocimetry apparatus (SCUVA). Case studies of jellyfish and other aquatic animals observed in the laboratory and in marine environments are subsequently interrogated using dynamical systems tools in order to quantitatively resolve the dynamics of animal swimming. The Lagrangian methods are shown to be readily extended to time-dependent measurements in three spatial dimensions and to in situ field measurements using a recently developed self-contained underwater velocimetry apparatus (SCUVA). Case studies of jellyfish and other aquatic animals observed in the laboratory and in marine environments are used to illustrate the proposed approach. We also show that predator-prey interactions during jellyfish swimming can be addressed using the aforementioned Lagrangian methods in combination with the Maxey-Riley equations for inertial particles in fluid flow.

1 This work was funded by NSF grant #0646573.

8:24AM A9.00003 Effects of hydrodynamic interactions in bacterial swimming,1, SUDDHASHIL CHATTOPADHYAY, Xiao Lun Wu, University of Pittsburgh — The lack of precise experimental data has prevented the investigation of the effects of long range hydrodynamic interactions in bacterial swimming. We perform measurements on various strains of bacteria with the aid of optical tweezers to shed light on this aspect of bacterial motility. Geometrical parameters recorded by fluorescence microscopy are used with theories which model flagella propulsion (Resistive force theory & Lighthill’s formulation which includes long range interactions). Comparison of the predictions of these theories with experimental data, observed directly from swimming bacteria, led to the conclusion that while long range interactions were important for single polar flagellated strains (Vibrio Alginolyticus & Caulobacter Crescentus), local force theory was adequate to describe the swimming of multi-flagellated Escherichia Coli. We performed additional measurements on E. Coli minicells (miniature cells with single polar flagellum) to try and determine the cause of this apparent effect of shielding of long range interactions in multiple flagellated bacteria.

1 Research supported by NSF Ocean Sciences and Energy for Sustainability

9:12AM A9.00005 Shape transformations and propulsion due to an elastic filament rotating in a viscous fluid, BIAN QIAN, THOMAS POWERS, KENNETH BREUER, Brown University — The deformation of an elastic filament in a viscous liquid is central to the mechanics of motility in cells ranging from E. coli to sperm. We use experiments and theory to study the shape transition of a flexible rod rotating in a viscous fluid and set at an angle to the axis of rotation. In the experiments, two modes of operation are studied: constant torque and constant speed, and the shape of the filament is measured using stereoscopic imaging. At low applied torque, the rod bends gently, while at high torque, the rod adopts a helical shape with the tip close to the axis of rotation. At constant torque, the transition from the splayed form to the helical form is abrupt, accompanied by a sharp increase in the rotational speed. As the torque is decreased, the shape change exhibits hysteresis, transitioning back to the splayed form at a lower torque. At constant speed, the transition is continuous characterized by a region of decreasing torque that persists until the transition to the helical form is complete. Calculations based on slender body and resistive force theory predict the torque-speed relationship and the filament shape throughout the entire operating range, and show excellent agreement with the experiments. The propulsive force is predicted to increase sharply after the shape transformation, at which point the efficiency is also predicted to reach a maximum.
9:24AM A9.00006 Propulsion by directional adhesion. JOHN BUSH, MANU PRAKASH, MIT — The rough, hairy integument of water-walking arthropods is well known to be responsible for their water-repellency; we here consider its additional propulsion role. We demonstrate that the tilted flexible leg hairs of water-walking arthropods render the leg cuticle directionally anisotropic: contact lines advance most readily towards the leg tips. The dynamical role of the resulting unidirectional adhesion is explored, and yields new insight into the manner in which water-walking arthropods generate thrust, glide and leap from the free surface. We thus provide new rationale for the fundamental topological difference in the roughness on plants and insects, and suggest novel directions for biomimetic design of smart, hydrophobic surfaces.

9:36AM A9.00007 The role of the ventral pedal waves in the locomotion of terrestrial gastropods, JANICE LAI, ROBERT D. SHEPHERD, JUAN C. DEL ALAMO, JAVIER RODRIGUEZ-RODRIGUEZ, JUAN C. LASHERAS, University of California San Diego — The locomotion of terrestrial gastropods exhibits unique characteristics which allow these animals to crawl on steep surfaces. Gastropods move by gliding over a ventral foot lubricated by mucus. The phasic movements of the foot produce periodic suction at its tips, which persist long after the foot has left the substrate. The present work develops an analytic model for the forcing of the ventral foot, producing a forward traction, while the rim of the foot adheres to the substrate and generates suction forces. We analyzed the kinematics and dynamics of locomotion by conducting two sets of experiments. In the first set, we used digital image processing to correlate the frequency and wavelength of the pedal waves to the migration velocity. In the second set, we computed the traction and adhesion forces produced by these animals from measurements of the deformation of an elastic substrate of known properties. We found that the strain energy exerted by the animal on the substrate is quasi-periodic, and explored a possible correlation between the mean speed of migration and the period of this energy fluctuation. In addition, we found that the pedal waves accelerate as they move forward along the ventral foot producing the symmetry break necessary for the generation of a net traction force.

1Partially supported by Spanish MEC (Fulbright Program)

9:48AM A9.00008 Flying, swimming and fluttering in 3D: potential flow around a rectangular deformable plate, CHRISTOPHE ELOY, LIONEL SCHOUVEILER, IRPHE, Marseille, France — The interaction between a flexible rectangular plate and the flow around it can serve as a model for several phenomena. This situation arises in many problems of animal locomotion as well as industrial ones such as airfoil flutter. So far, most models have assumed a 2D problem for the sake of simplicity. We show here how to extend these models to include the finite plate aspect ratio in the analysis. We consider a rectangular deformable plate moving in a uniform flow at small amplitude such that the plate and its wake remain in the same plane at first order. The potential flow around the plate is calculated in the Fourier space and then averaged along the span. The result is a new integral equation for the vorticity distribution both inside the solid plate and in its wake. It means that the 3D effects can be taken into account by simply modifying the potential of a point-vortex (or equivalently the Green function of the Laplace’s equation).

2This work received financial support from the French ANR project DRAPEAU

10:00AM A9.00009 Symmetry breaking in gastropod locomotion through acceleration or deceleration of the pedal waves, JUAN C. DEL ALAMO, JAVIER RODRIGUEZ-RODRIGUEZ, JANICE LAI, ROBERT D. SHEPHERD, JUAN C. LASHERAS, University of California San Diego — Marine and terrestrial gastropods move by gliding over a ventral foot that is lubricated by secreted mucus (terrestrial) or simply by water (marine). The rim of the ventral foot generates suction forces that keep the animal adhered to the substrate. The central part of the foot produces a forward traction force by generating trains of pedal waves through periodic muscle contractions. Recent experiments show that, in some gastropods, these pedal waves become faster and longer as they move forward, suggesting a mechanism for breaking the symmetry in the flow between the pedal waves and the substrate. To investigate this mechanism, we have analyzed theoretically a two-dimensional lubrication layer between a train of waves of slowly varying length and speed, and a flat, rigid, impermeable surface. The inhomogeneity of the pedal waves has been modeled through multiple-scale asymptotics. We have considered a Newtonian fluid to separate the effect of this inhomogeneity from the viscoelastic symmetry breaking reported in previous works.

1Partially supported by Spanish MEC (Fulbright Program)

10:12AM A9.00010 The unsteady flow over a bat wing in mid-downstroke, FLORIAN MUJRES, CHRISTOFFER JOHANSSON, RYAN BARFIELD, MARTA WOLF, Lund University, GEOFFREY SPEDDING, University of Southern California, ANDERS HEDENSTROM, Lund University — Birds, bats and insects have provided inspiration for human-designed small-scale flying machines, and while insects have long been known to rely on unsteady separated flows for their above-average aerodynamic performance at small-scale, the details of air flows over bird and bat wings have been harder to elucidate, mainly because of the extra complexity and precautions required in live experiments. Here we report on the first experiments of the airflow around a bat wing in free (but trained) flight in a low-turbulence wind tunnel. The aerodynamics of fixed wings at these Reynolds numbers are notoriously sensitive to small disturbances of the initially laminar, attached boundary layer, but these flight experiments show that the instantaneous flow fields around the flapping wing bear almost no resemblance to an equivalent fixed-wing experiment. The circulation increment due to the presence of a strong leading-edge vortex is estimated to provide a significant fraction of the total lift. Implications for the design and control of micro-air vehicles are considered.

10:24AM A9.00011 Mechanics of Mammalian Swimming, TIMOTHY WEI, PAUL LEGAC, Rensselaer Polytechnic Institute, FRANK FISH, West Chester University, TERRIE WILLIAMS, University of California. Santa Cruz, RUSSELL MARK, USA Swimming, SEAN HUTCHISON, King Aquatics — Propulsion of large mammals (i.e. dolphins and humans) has been of great interest for both technological and athletic reasons. The fundamental question is how fast can a mammal swim? Digital Particle Image Velocimetry (DPIV) has been modified to be safely used on swimmers and dolphins. Experiments of dolphins performing various swimming behaviors were performed at the Long Marine Laboratory, University of California, Santa Cruz. Vortices generated by the dolphins’ tail motions were used to estimate thrust production. Also, a two-dimensional dynamic force balance was constructed to study and improve the mechanics of elite swimmers. Paired with an underwater video camera, the forces seen could be directly related to the motion of the swimmer. These force measurements could be correlated to time resolved DPIV measurements of flow around the swimmers. Measurements made with swimmers, Megan Jendrick (2000 Olympic gold medalist) and Ariana Kukors (4x US National Champion), as well as data from trials with two dolphins will be presented.

10:36AM A9.00012 Synchronization and hydrodynamic interactions, THOMAS POWERS, BIJAN QIAN, KENNETH BREUER, Division of Engineering, Brown University — Cilia and flagella commonly beat in a coordinated manner. Examples include the flagella that Volvox colonies use to move, the cilia that sweep foreign particles up out of the human airway, and the nodal cilia that set up the flow that determines the embryonic axis in developing vertebrate embryos. In this talk we present an experimental study of how hydrodynamic interactions can lead to coordination in a simple idealized system: two nearby paddles driven with fixed torques in a highly viscous fluid. The paddles attain a synchronized state in which they rotate together with a phase difference of 90 degrees. We discuss how synchronization depends on system parameters and present numerical calculations using the method of regularized stokeslets.
10:48 AM A9.00013 An experimental and numerical study of fluid flow generated by a single nodal cilium. XINGZHOU YANG, Center for Computational Science, Tulane University, LISA FAUCI, Department of Mathematics, Tulane University, ARSHAD KUDROLLI, Department of Physics, Clark University — A rotating nodal cilium is said to generate fluid flow in the node of a developing embryo by posterior tilt leading to the left-right asymmetry of the mammalian body. In order to develop a physical understanding of the fluid generated and the effect of the enclosing chamber, we perform scaled-up fluid-mechanics experiments and numerical simulations using the method of Regularized Stokeslets for zero Reynolds number. Important mechanical parameters, such as the geometry of the rods, dimensions of the tank, and the ratio of viscous to elastic stresses can be scaled to match typical cilia and cell. Digital imaging and tracer particle tracking techniques are used to measure the location and shape of the rods and the fluid flow. We will discuss the nature of the hydrodynamic velocity fields which are found to be more complex than anticipated by previous studies.

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A10 DMP: Tunneling on Cuprate Superconductors Morial Convention Center R08

8:00AM A10.00001 Local tunneling probe of low-energy Andreev states on (110) $Y_{0.95}Ca_{0.05}Ba_2Cu_3O_{7-\delta}$ thin films in an applied magnetic field$^1$, J.H. NGAI, Department of Physics, University of Toronto, Toronto, Canada, R. BECK, G. LEIBOVITCH, G. DEUTSCHER, Department of Physics and Astronomy, Raymond and Beverly Sackler faculty of Exact Sciences, Tel Aviv University, Tel Aviv, Israel, J.Y.T. WEI, Department of Physics, University of Toronto, Toronto, Canada — Cryomagnetic scanning tunneling spectroscopy (STS) was performed on (110)-oriented $Y_{0.95}Ca_{0.05}Ba_2Cu_3O_{7-\delta}$ thin films, in order to reveal coherence-length scale information on the symmetry of the high-$T_c$ order parameter (OP) in a magnetic field. In zero-field at 4.2K, both spontaneously split and unsplit zero-bias conductance peaks (ZBCP) are seen in the STS spectrum. The two types of peak spectra exhibit increasing splitting in a field applied along the c-axis of the film. Both spontaneous and field-induced ZBCP splitting indicate a lifting in the degeneracy of the low-energy Andreev states, consistent with time-reversal symmetry breaking. These results are discussed within the context of the Doppler effect as well as intrinsic vs. field-induced complex components in the high-$T_c$ OP.

$^1$This work was supported by NSERC, CFI/OIT and the Canadian Institute for Advanced Research.

8:12AM A10.00002 Magnetic-field effect on the quasiparticle excitation observed by the tunneling spectroscopy in $Bi_2Sr_2CaCu_3O_{8+\delta}$ single crystal$^2$, YI XUAN, Texas Center for Superconductivity at the University of Houston, H.J. TAO, Z.Z. LI, B.R. ZHAO, Z.X. ZHAO, National Laboratory for Superconductivity, Institute of Physics and Center for Condensed Matter Physics, Chinese Academy of Sciences, China — In the d-wave superconductor, due to the existence of nodes of the pairing gap, the field-dependence of the quasiparticle density of state has been predicted to be essentially different from the behavior in the s-wave case $^1$. Here we report the planar junction tunneling spectra at different magnetic fields in the high-$T_c$ superconductor $Bi_2Sr_2CaCu_3O_{8+\delta}$ to study how the field modifies the quasiparticle excitation. $^1$G. E. Volovik, JETP Lett. 58, 469 (1993).

$^2$This research has been supported by the National natural Science Foundation of China under Grant No. 19974070.

8:24AM A10.00003 Role of competing orders (COs) in the low-energy pseudogap (PG) phenomena and quasiparticle (QP) excitations of hole- and electron-type cuprate superconductors$^1$. A.D. BEYER, M.S. GRINOLDS, M.L. TEAGUE, N.-C. YEH, Phys. Dept., Caltech, Pasadena, CA, S.-I. LEE, Phys. Dept., Pohang U., Korea — Our cryogenic scanning tunneling spectroscopic studies of spatially resolved QP density of states (DOS) in hole-type $YBa_2Cu_3O_7$ and electron-type $La_{2-\delta}Sr_{1.9}CuO_4$ cuprate superconductors (SC) reveal that the existence of COs in the cuprates can account for many seeming non-universal phenomena. Namely, we analyze the low-energy QP excitation spectra by using a microscopic model of coexisting SC/CO, with density-wave type COs, and find that various spectral characteristics are uniquely determined by the parameters $\Delta_{SC}$, $V_{CO}$, $Q$, and $\Gamma$ ($\Delta_{SC}$: SC gap, $V_{CO}$: CO gap, $Q$: CO wave-vector, $\eta$: strength of quantum fluctuations, $\Gamma$: line-width of QP spectral peak). For instance, $V_{CO} > \Delta_{SC}$ ($V_{CO} \leq \Delta_{SC}$) in hole- (electron-) type cuprates can account for the presence (absence) of the low-energy PG. Anomalous momentum-dependent QP properties such as the Fermi arcs and antiferromagnetic hot spots can also be explained. In finite magnetic fields, the QP DOS inside the vortex core of both types of cuprates reveal unconventional PG-like features at energies comparable to the $V_{CO}$ values derived by our analysis.

$^1$The work at Caltech was supported by NSF Grant DMR-0405088.

8:36AM A10.00004 Spatially Resolved Quasiparticle (QP) Spectra in the Vortex State of Electron-Type Cuprate Superconductor (SC) $La_{1.1}Sr_{0.9}CuO_2(La-112)$, M.L. TEAGUE, A.D. BEYER, M. GRINOLDS, N.-C. YEH, Phys Dept Caltech Pasadena, CA, S.I. LEE, Pohang U., Korea — The low-energy excitations of cuprate superconductors are unconventional and are susceptible to changes in temperature, doping and magnetic field. Our recent experiments and microscopic theoretical analysis suggest that these phenomena may be attributed to the presence of competing orders (COs) and strong quantum fluctuations. Here we present our scanning tunneling spectroscopic studies that support coexisting SC/CO in La-112, an optimally doped electron-type cuprate with $T_c=43$ K. In zero-field, the histogram of the QP spectra at 9 K over an (100x100) nm$^2$ area reveals a single set of spatially homogeneous peaks at $\Delta_{eff} = 11.8 \pm 1.5$ meV. Our analysis of the data (with two energy gaps of SC and CO, $\Delta_{SC}$ and $V_{CO}$) suggests $\Delta_{eff} = (\Delta_{SC} + V_{CO})^2/\Delta_{SC}$ and the presence of quantum fluctuations. With increasing magnetic field to 6 Tesla, $\Delta_{eff}$ shifts downward to 10.0 meV due to the overall suppression of $\Delta_{SC}$, and the spatial variation of the spectra are consistent with vortex periodicity. Moreover, pseudogap-like spectral features occur at $\Delta_{eff}$ inside the vortex cores while the spectra outside the vortex cores retain a gap value at $\Delta = \pm \Delta_{eff}$. This work was supported by NSF Grant DMR-0405088.
8:48AM A10.00005 Importance of matrix element effects in the scanning tunneling spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 + \delta$\textsuperscript{1}, ARUN BANSIL, Northeastern University, JOUKO NIEMINEN, TUT, Finland and Northeastern University, ROBERT MARKIEWICZ, HSIN LIN, Northeastern University — Scanning tunneling microscopy/spectroscopy (STM/STS) techniques have entered the realm of high-Tc’s impressively by offering atomic scale real space resolution and meV resolution in bias voltages. STM/STS spectra, however, represent a complex mapping of electronic states of interest related to the CuO2 planes, since the tunneling current must reach the tip after being filtered through the overlayers (e.g. SrO and BiO in Bi2212). We have developed a Green function approach for realistic modeling of STM/STS spectra of the cuprates, where the tunneling current is evaluated directly including the effect of overlayers, with all orbitals within a few eV’s of the Fermi energy $E_F$ accounted for. Our calculations show the presence of strong matrix element effects, which lead to significant differences between the d1/dv spectra and the local density of states (LDOS) of CuO2 planes. For instance, the $d_{x^2-y^2}$ signal is found to be dominated by non-vertical hopping between the CuO2 and BiO layers. A substantial electron-hole anisotropy of the tunneling spectrum, which is in accord with experiments, is naturally explained by the contribution from $d_{x^2}$ and other orbitals below $E_F$.

\textsuperscript{1}Work supported in part by the USDOE.

9:00AM A10.00006 Temperature dependent Scanning Tunneling Spectroscopy of impurities in Bi2Sr2CuO6+$\delta$ through the transition temperature, KAMALESH CHATTERJEE, DOUGLASS WISE, MICHAEL BOYER, MIT, TAKESHI KONDO, TSUNEHIRO TAKEUCHI, HIROSHI IKUTA, YAYU WANG, ERIC HUDSON, MIT — Scanning Tunneling Microscopy has been used to study detailed electronic spectrum in atomic scale defects in high temperature superconductors. We present Scanning Tunneling Spectroscopy of impurities in Bi2Sr2CuO6+$\delta$ (Bi-2201) over a wide range of temperatures. Surprisingly, native impurity resonances, similar to the ones previously observed in Bi2Sr2CaCu2O8+$\delta$ (Bi-2212), spatially coexist with the superconducting gap at low temperatures and survive almost unchanged through the superconducting transition temperature $T_c$. We shall discuss the implications of these findings on the relationship between superconducting gap and pseudogap in these materials.

9:12AM A10.00007 Visualizing Two Gaps in the High Temperature Superconductor Bi-2201, MICHAEL BOYER, W.D. WISE, KAMALESH CHATTERJEE, MIT, MING YI, Stanford U., T. KONDO, Ames, T. TAKEUCHI, H. IKUTA, Nagoya U., E.W. HUDSON, MIT — The relationship between the superconducting and pseudogap states in the cuprates has been a subject of much interest as well as debate in the HTS community. At the forefront of this debate is whether the pseudogap exists below $T_c$, and if it does, in what capacity. We present scanning tunneling microscopy measurements which provide evidence for two distinct but simultaneously coexisting gaps in the density of states of Bi2Sr2CuO6+$\delta$ (Bi-2201) below $T_c$; one identified as the superconducting gap and the other, the pseudogap. In addition, we discuss our preliminary doping dependence measurements showing that the small (superconducting) gap scales with $T_c$ while the larger (pseudogap) gap scales with $T^{*}$ indicating a consistency with their identification.

9:24AM A10.00008 Temperature and doping dependent FT-STS studies of Bi-2201, WILLIAM WISE, KAMALESH CHATTERJEE, MICHAEL BOYER, YAYU WANG, Massachusetts Institute of Technology, TAKESHI KONDO, Ames Laboratory, TSUNEHIRO TAKEUCHI, HIROSHI IKUTA, Nagoya University, ERIC HUDSON, Massachusetts Institute of Technology — We present Fourier transform scanning tunneling spectroscopy (FT-STS) results in superconducting Bi-2201. The data presented are drawn from samples at a variety of dopings, and from experiments both below and above the superconducting transition temperature $T_c$. A number of unexpected trends are revealed by this systematic study. We interpret the results in light of several theories and make comparisons to results from other crystal systems.

9:36AM A10.00009 Bogoliubov angle and visualization of particle-hole mixture in superconductors, KAZUHIRO FUJITA, Cornell University, ILYA GRIGORENKO, Los Alamos National Laboratory, JINHO LEE, MIAO WANG, Cornell University, JIAN XIN ZHU, Los Alamos National Laboratory, J.C. DAVIS, Cornell University, Brookhaven National Laboratory, HIROSHI EISAKI, AIST, Tsukuba, SHIN-ICHI UCHIDA, The University of Tokyo, ALEXANDER V. BALATSKY, Los Alamos National Laboratory — We propose a new technique to visualize particle-hole mixture in high temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, using the Spectroscopic Imaging Scanning Tunneling Microscopy (SI-STM). Depending on the polarity of bias voltage, SI-STM can sample the particle and hole content of a superconducting excitation, Bogoliubov quasi-particle. 'Bogoliubov angle' (BA) is a measure of the relative weight of particle and hole amplitude in the Bogoliubov quasiparticle, which is determined by taking ratio of the differential conductance at positive and negative biases. BA allows one to measure directly the energy and position dependent particle-hole admixture and therefore visualize robustness of superconducting state locally. We will demonstrate the power of this new technique and discuss the momentum space (q-space) electronic structure in the talk.

9:48AM A10.00010 Phase-sensitive scattering of Bogoliubov quasi-particles in (Ca,Na)$_2$CuO$_2$Cl$_2$ under magnetic field, T. HANAGURI, Y. KOHSAKA, M. ONO, RIKEN (Inst. Phys. and Chem. Research), M. MALTESEVA, P. COLEMAN, Dept. of Phys. and Astronomy, Rutgers Univ., I. YAMADA, M. AZUMA, M. TAKANO, Inst. Chem. Research, Kyoto Univ., K. OHISHI, Japan Atomic Energy Agency, H. TAKAGI, RIKEN/Univ. Tokyo — Magnetic-field effect on the quasi-particle interference (QPI) in Ca$_{1.86}$Na$_{0.14}$CuO$_2$Cl$_2$ ($T_c \sim 25$ K) has been studied using Fourier-transform spectroscopic-imaging scanning tunneling microscopy. In the absence of magnetic field, all scattering vectors expected from the octet model for QPI [1] were detected in the Fourier-transformed conductance-ratio maps [2]. We have found that magnetic field enhances (suppresses) the amplitude of the standing waves due to QPI if the signs of the d-wave superconducting order parameter in momentum space are the same (different) between initial and final states of the scattering. We interpret the results in light of several theories and make comparisons to results from other crystal systems.


10:00AM A10.00011 Evolution of the electronic excitation spectrum with strongly diminishing hole-density in superconducting Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, J.W. ALLDREDGE, JINHO LEE, Cornell University, K. MCELROY, University of Colorado, M. WANG, K. FUJITA, Cornell University, Y. KOHSAKA, Magnetic Materials Laboratory, RIKEN, C. TAYLOR, Cornell University, H. EISAKI, NI-AIST, S. UCHIDA, University of Tokyo, P.J. HIRSCHFELD, University of Florida, J.C. DAVIS, Cornell University — We use tunneling spectroscopy to measure the $T>$0 spectrum of electronic excitations N(E) over a wide range of hole-density in superconducting Bi2212. We introduce a parameterization for N(E) based on an anisotropic d-wave energy-gap plus an effective scattering rate which varies linearly with energy. We demonstrate that this form of N(E) allows successful fitting of differential tunneling conductance spectra throughout much of the Bi2212 phase diagram. A single, particle-hole symmetric, anisotropic energy-gap, in combination with a strongly energy dependent effective scattering rate, can describe the excitations without recourse to an additional energy gap of another ordered state. However we also observe two distinct and diverging energy scales in the system: the energy-gap maximum $\Delta_1$, and a lower energy scale $\Delta_0$ separating the spatially homogeneous and heterogeneous electronic structures.
10:12AM A10.00012 Temperature Evolution of Local Pairing & Electron-Boson Coupling in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$. KENJIRO K. GOMES, ABHAY PASUPATHY, AAKASH PUSHP, COLIN PARKER, Department of Physics, Princeton University, GENDA GU, Brookhaven National Laboratory, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, ALI YAZDANI, Department of Physics, Princeton University — Recently, we have shown using variable temperature scanning tunneling microscopy measurements that the pairing in Y-Ba-Cu-O superconductors Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$ persists in nanoscale regions at temperatures above $T_c$. [1] Using the ability to track the same atomic location with temperature, we have examined the evolution of the electronic states from well below $T_c$ to above the temperature at which the pairs first form locally. We will present these results for an overdoped sample. Using these measurements we extract the evolution of the pairing gap with temperature and show that pairing gaps at different atomic sites close at different temperatures. Our technique also allows us to quantitatively analyze the local electron-boson coupling for different atomic sites with different pairing strengths. Our results show that there is no connection between the variation of the gap magnitude and the bosonic mode associated with the “dip-hump” feature in the spectra. [1] Gomes et al. Nature 447, 569–572 (2007).

1Work supported by NSF, DOE and PCCM-MRSEC.

10:24AM A10.00013 Electronic Origin of the Nanoscale Variation of Pairing Gaps in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$. ABHAY PASUPATHY, KENJIRO K. GOMES, AAKASH PUSHP, COLIN PARKER, Department of Physics, Princeton University, GENDA GU, Brookhaven National Laboratory, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, ALI YAZDANI, Department of Physics, Princeton University — The magnitude of the low-temperature superconducting gap measured in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$ shows large nanoscale spatial variations. On raising the temperature, these superconducting gaps disappear locally at temperatures above the superconducting transition temperature $T_c$. We present the first atomically resolved measurements of the spectrum of overdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$ at temperatures where all gaps have closed. We show that the shape of this “normal” state spectrum is inhomogeneous over a length scale similar to that of the gap variation at low temperature. We then track the same lattice sites down to low temperature and observe the opening of gaps in the spectrum. We will discuss the relationship between the shape of the spectrum measured in the “normal” state at high temperature and the size of the low-temperature superconducting gap at the same atomic site.

1Work supported by NSF, DOE and PCCM-MRSEC.

10:36AM A10.00014 Temperature Evolution of the Electronic States & Multiple Gap Features in Bi$_2$Sr$_{2-y}$La$_y$CuO$_6$+$\delta$. AAKASH PUSHP, ABHAY PASUPATHY, KENJIRO K. GOMES, COLIN PARKER, Department of Physics, Princeton University, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, ALI YAZDANI, Department of Physics, Princeton University — Like Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$, Bi$_2$Sr$_{2-y}$La$_y$CuO$_6$+$\delta$ samples show inhomogeneous gaps in the DOS at low temperature. We present atomic resolution STM spectroscopy measurements of the evolution of the DOS with temperature for optimal ($y$=0.4) and overdoped ($y$<0.4) samples and compare these measurements to Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$. In Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$+$\delta$, the low temperature ($T$< $T_c$) spectra of overdoped samples are all characterized by a single d-wave gap with sharp coherence peaks. In contrast, Bi$_2$Sr$_{2-y}$La$_y$CuO$_6$+$\delta$ shows a variety of spectra at low temperature ranging from those with gaps to ones with multiple gap features [1]. By measuring the temperature evolution of these gap features at given lattice sites for various doping levels, we estimate the local temperature at which pairing develops in these samples. [1] Boyer et al., Nat Phys 3, 802 (2007)

1Work supported by NSF, DOE and PCCM-MRSEC.

10:48AM A10.00015 Local Signatures and Spectral Inversion of Bosonic Mode Coupling in a High-Temperature Superconductor. LAILA S. MATTOS, CHRISTOPHER R. MOON, BRIAN K. FOSTER, GABRIEL ZELTZER, MARTIN GREVEN, HARI C. MANOHARAN, Stanford University — High-resolution spectroscopy and mapping of the high-temperature superconductor Bi$_2$Sr$_2$Ca$_{0.93}$Y$_{0.07}$Cu$_{2+x}$d was performed with a custom-built low-temperature scanning tunneling microscope. At optimal doping ($T_c$ ∼ 96 K), these materials exhibit unusually strong spectral sidebands characteristic of electron-boson coupling. The magnitude of these Holstein-like d-wave density of states replicas facilitates a spectral inversion procedure, from which the critical parameters of the bosonic coupling can be directly extracted. This results in electron-boson coupling $\lambda$ ∼ 0.2-0.4 and boson energy $\Omega$ ∼ 70-90 meV. Origins and implications of these excitations will be discussed.

1Supported by DOE, NSF, and ONR.

Monday, March 10, 2008 8:00AM - 11:00AM – Session A11 DMP: Focus Session: MgB2-like: Exotic Behavior in MgB2-like Materials Morial Convention Center RO9

8:00AM A11.00001 High quality MgB$_2$ thin films in clean and dirty limit realized via HPCVD. CHENGANG ZHUANG, SHENG MENG, QINGRONG FENG, ZIZHAO GAN, PKU P.R.C, HUAN YANG, YING JIA, HAIHU WEN, CAS P.R.C, XIAOXING XI, PSU USA — Pure and carbon-doped MgB$_2$ thin films are fabricated using hybrid physical-chemical vapor deposition. Excellent properties are obtained in the pure samples, including $T_c$ = 41.4K, $\rho$(42K)$\sim$0.3 $\mu$ $\Omega$ cm, which indicates that films are in the clean limit. Ultrahigh critical current density, up to $1\times10^5$A/cm$^2$ at 5K and zero fields, approaching the theoretical deparing critical of MgB$_2$, was observed in a 150nm-wide microbridge, in agreement with the results derived using a Bean Model from the magnetization measurements. Large normal state magnetoresistance before the transition, about 40% at 7T, and absence of flux jump at low temperature and low field regions in the magnetization curves strongly support that the film is very clean. To enhance upper critical field and flux pinning, carbon doping is employed and realized in a dual-heater HPCVD setup from the thermal decomposition of CH$_4$, $\mu_0$H$_{2}$(0)$\sim$54T, $J_c$(5K,6T)$\sim$3$\times$10$^5$A/cm$^2$, as well as $T_c$(0)$\sim$34K and $\rho$(42K)$\sim$47$\mu$ $\Omega$.cm are achieved in the carbon-doped films. By controlling the carbon concentration, MgB$_2$ films in dirty limit can be prepared.

1This work was supported by the NSF No. 50572001 and the 973 project: 2006CD601004.
8:12AM A11.00002 Superconducting properties of MoN microfibers and thin films

A. Karki, LSU Department of Physics and Astronomy, EDEM OKUDZETO, LSU Department of Chemistry, PHIL ADAMS, DAVID YOUNG, LSU Department of Physics and Astronomy — We present the superconducting transport properties measurements on polycrystalline MoN synthesized in the form of thin films and microfibers. The samples were prepared by heating Mo films and Mo-coated carbon fibers to temperatures between 850 °C and 1000 °C for different time periods in a flowing stream of ammonia (NH₃) gas under atmospheric pressure. The microfibers and thin films had a transition temperature Tc ~ 12.2 K, which is substantially higher than the first reported room temperature superconductor MoB. A high pressure furnace, using a 19 mm truncation edge length, cubic anvil capable of reaching 3.3 GPa and 2000 °C was used to grow crystals of MgB₂-O-duty coating carbon fibers grown by other methods. We also present critical current measurements on microfibers which consisted of a 50-nm thick layer of polycrystalline MoN synthesized directly onto 5 micron-diameter carbon fibers. The microfibers supported current densities in excess of 10⁷ A/cm² well below Tc. Near Tc, Jc was well described by the power law [1-(T/Tc)²]¹/².

1 NSF DMR 04-49022

8:24AM A11.00003 Theory of Raman Scattering from Leggett’s Collective Mode in a Multiple Band Superconductor: Application to MgB₂

Miles Klein, University of Illinois at Urbana-Champaign — Using an extension of BCS theory to a two-band superconductor, Leggett showed that if the relevant parameters obeyed certain conditions a collective mode would exist corresponding to the counter flow of the two condensates. I have extended earlier work on electronic Raman in superconductors to the multiple band case in order to incorporate Leggett’s theory. The following effects have been included: (a) Vertex correction in the particle/hole channel where the Raman vertex acts. (b) Realistic parameters that apply to MgB₂ yielding a counter flow mode that decays into the pair-breaking continuum associated with the lower gap π band. (c) Large finite wave-vector effects due to the relatively large Fermi velocity of the π band. (d) Integration over the wave-vector in part (c) necessitated by the exponential decay of the photon fields traveling into and out of the metallic sample. A comparison to the results of Blumberg will be given. A. J. Leggett, Progr. Theor. Phys. 36, 901 (1966). M.V. Klein and S.B. Dierker, Phys. Rev. B29, 4976 (1984). G. Blumberg et al., Phys. Rev. Lett. 99, (2007); arXiv:0710.2803.

8:36AM A11.00004 MgB₂: Novel properties due to multibands

Girsh Blumberg, Laboratory, Alcatel-Lucent — About 40 years ago A.J. Leggett proposed a new collective mode arising from cross-tunneling of Cooper pairs residing on different Fermi surfaces of a multiband superconductor: Leggett’s collective mode is caused by a counter flow of the interacting superfluids leading to small fluctuations of the relative phase of the condensates while the total electron density is locally conserved. Here we present direct spectroscopic observation of the Leggett’s excitation in the MgB₂ superconductor containing two pairs of Fermi surfaces resulting from π- and σ-bands. Electronic Raman scattering studies have revealed three distinct superconducting (SC) features: (i) a clean threshold of Raman intensity at 4.6 meV consistent with the π-band SC gap; (ii) the SC pair breaking coherence peak at 13.5 meV consistent with excitations above the superconducting (SC) features; (iii) a broad threshold at 5.5 meV consistent with the σ-band SC gap. A comparison to the results of Blumberg will be given. A. J. Leggett, Progr. Theor. Phys. 36, 901 (1966). M.V. Klein and S.B. Dierker, Phys. Rev. B29, 4976 (1984). G. Blumberg et al., Physica (Amsterdam) 456C, 75 (2007).

9:12AM A11.00005 Microwave properties of epitaxial MgB₂ films and micro-bridges

M.V. Costache, G.X. Miao, J.S. Moodera, Massachusetts Institute of Technology — The high transition temperature and simple AlB₂ structure make the MgB₂ superconductor a promising new material for application in superconducting electronic devices. In order to reach this goal, in addition to the development of MgB₂ Josephson Junctions (JJ), we have explored the superconducting properties of lithographically patterned micro sized bridges in high quality epitaxial MgB₂ films. These thin film micro size wire bridges show JJ characteristics. The current-voltage (I-V) characteristics show the expected JJ behavior as a function of temperature, magnetic field and microwave radiation including hysteresis. Large change in the hysteresis behavior is observed when the microwave power is varied. The large hysteretic I-V can have potential as a memory element. The details will be discussed.

9:24AM A11.00006 Force-Detected NMR Study of Single-Crystal MgB₂ using Ultrasonic Oscillators

Han-Jong Chia, Mark Monti, Samaresh Guhhaia, John Markert, Physics, University of Texas at Austin, JAE-Hyuk Choi, Mechanical Metrology Group, Division of Physical Metrology, KRISS, Korea, Sung-Ik Lee, Pohang University, Korea — MgB₂ is a unique superconductor with a relatively high T_c and two nearly independent electronic bands. An NMR study of ¹¹B in MgB₂ using polycrystalline samples [1] did not observe any two-band effects, nor a Hebel-Slichter coherence peak, possibly due to large H₂ anisotropy (and thus a distribution of T_c’s). Anisotropic NMR studies of MgB₂ have proven difficult due to the small size (~ 10 μm) of high-quality crystals. A large-single-crystal conventional NMR study [2] could not probe the superconducting state due to line broadening. We have set out to use the exquisite sensitivity of Nuclear Magnetic Resonance Force Microscopy (NMRFM) to probe the behavior of ¹¹B in single crystal MgB₂. We have fabricated ultrasonic mechanical oscillators using e-beam lithography to facilitate detection of the weak ¹¹B resonance; these have resonance frequencies of 1–10 kHz, spring constants of ~ 10⁹ N/m, and quality factors >3000 at 77 K. We report our initial detection of the ¹¹B nuclear resonance and our plans to study relaxation rates in single crystal MgB₂ [1] H. Kogawa et al., Phys. Rev. Lett. 87, 127001 (2001). [2] S. Strässle et al., Physica C 1046, 166 (2007). *Supported by NSF DMR-0605828 and DOE-0549147.

9:36AM A11.00007 High pressure synthesis of single crystalline MgB₂

M. Tillman, Ames Lab / Iowa State University, G. Lapertot, CEA-Grenoble, DFRMC/SPSMS/IMAPEC, R. Prozorov, C. Martin, S.L. Bud’ko, P.C. Canfield, Ames Lab / Iowa State University — We report the results of single crystal growth of MgB₂. A high pressure furnace, using a 19 mm truncation edge length, cubic anvil capable of reaching 3.3 GPa and 2000 C was used to grow crystals of MgB₂ out of the Mg-B-N ternary. Design, setup, and calibration will be discussed as well as correlations between pressure and temperature profiles and crystal size. Results of measurements of penetration depth and H₂(T) on single crystals will be shown as well as the results of initial doping studies.

3 Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.
9:48AM A11.00008 Electric-field-effect studies of atomically thin flakes of superconducting NbSe\textsubscript{2} prepared by mechanical exfoliation. NEAL STALEY, JAIN WU, PETER EKLUND, YING LIU, Pennsylvania State University, LINJUN LI, ZHUAN XIU, Zhejiang University, China — Recent years have yielded many studies on electric field modulated superconductivity. In order to achieve the high carrier density changes needed to modulate superconductivity, two main approaches have been tried, ultra thin films grown by in situ quench deposition or few-layer single crystalline films of superconductors grown by pulsed laser deposition or molecular beam epitaxy. However in both cases, difficulties have been encountered, ultra thin films are subject to large amounts of disorder, and it is difficult if not impossible to grow single layered superconductors. Using a simple micromechanical exfoliation technique, we are able to create single crystal single layered graphite, featuring a linear density of states, allowing its physical properties to be tuned by gate voltage. Using this mechanical exfoliation procedure we fabricated ultra thin single crystalline NbSe\textsubscript{2} flakes ranging from double layered to many layered as estimated using an optical technique correlated to AFM and Raman spectroscopy measurements. Using a lithography-free, “all dry” process we fabricated devices showing modulated $T_c$ with applied gate voltage as well as a superconductor insulator transition tuned by the number of layers.

10:00AM A11.00009 Low Energy Electronic Structure of an Excitonic CDW Melted Novel Superconductor\textsuperscript{1}, DONG QIAN, DAVID HSIEH, LEWIS WRAY, YUQI XIA, Physics Department, Princeton University, E. MOROSAN, R.J. CAVA, Chemistry Department, Princeton University, M.D. HASAN, Physics Department, Princeton University — A superconducting (SC) state has very recently been observed upon successful doping of the charge-density wave (CDW) ordered triangular lattice TiS\textsubscript{2} with copper. Using angle-resolved photoemission spectroscopy (ARPES) we studied the doping evolution of the electronic structure of Cu\textsubscript{x}TiS\textsubscript{2}. The momentum space locations of the doped electrons that form the Fermi sea of the parent superconductor is identified. With increasing electron doping, we observe a significant rise of chemical potential which is found to destabilize the long range CDW order. At the same time the emergence of a large density of states in the form of a narrow electron pocket near the $k$-points of the Brillouin zone favors the onset of superconductivity within the BCS-Eliashberg scenario. With doping, we find that the kinematic nesting volume increases whereas the coherence of the CDW order sharply drops. The $k$-space electron distributions highlight the unconventional interplay of CDW to SC cross-over achieved through non-magnetic copper doping.

\textsuperscript{1}This work is supported by DOE Grant No. DEFG-02-05ER46200 and NSF Grant No. DMR-0213706.

10:12AM A11.00010 Sandwich-type MgB\textsubscript{2} tunnel junctions\textsuperscript{1}, KE CHEN, YI CUI, QI LI, XIAOXING XI\textsuperscript{2}. Department of Physics, The Pennsylvania State University, University Park, Pennsylvania, USA — Properties of superconductors, such as band gap, density of states (DOS) of quasiparticles, and effective phonon spectra, can be studied by electrical tunneling with a high energy resolution of several $\hbar\omega_{\text{ph}}$. Sandwich-type MgB\textsubscript{2} tunnel junctions with Pb or Ag as the counter-electrodes were made on Hybrid Physical-Chemical Vapor Deposition MgB\textsubscript{2} films with thermal oxide tunnel barrier. The tunnel junctions exhibit very small subgap current at 4.2 K. Fit to the BCS DOS relation, the $\sigma$-band and $\tau$-band gaps of MgB\textsubscript{2} are found to be 2.3 and 7.4 meV at 4.2 K respectively. Josephson tunneling was observed with $I_{J\text{rms}}$ product following the BCS temperature dependence relation, and the critical current showing a Fraunhofer pattern modulated by the applied magnetic field. Effective phonon modes are revealed at 42, 61, and 74 meV. These superb tunnel junctions give us deep insights into the properties of MgB\textsubscript{2}.

\textsuperscript{1}The work is supported by ONR. We appreciate helpful discussions with John Rowell and Jochen Geerk.
\textsuperscript{2}Also with Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA

10:24AM A11.00011 Hybridized Abrikosov Flux-lines and Pancake Vortices in Two-band Superconductors with Mixed Dimensionality\textsuperscript{1}, K. TANAKA, Department of Physics and Engineering Physics, University of Saskatchewan, M. ESCHRICHT, Instituf fuer Theoretische Festkoerperfisik, Universitaet Karlsruhe — We study electronic structure and thermodynamic properties of a two-band superconductor, in which one band is ballistic and quasi-two dimensional (2D), and the other is diffusive and three dimensional (3D). We assume that superconductivity in the 3D diffusive band is “weak”, i.e., mostly induced, as is the case in MgB\textsubscript{2}. Hybridization with the “weak” 3D diffusive band has significant and intriguing influence on the electronic properties of the “strong” 2D ballistic band. In particular, the effects of Coulomb interactions in the diffusive band and unusual Kramer-Pesch effect are excluded. Furthermore, based on a circular-cell approximation within the quasiclassical theory of superconductivity, we explore the effects of magnetic field on vortex structure in such a two-band superconductor. We discuss hybridization of Abrikosov flux lines in the 3D diffusive band with pancake vortices in the 2D ballistic band.

\textsuperscript{1}NSERC of Canada, Canada Foundation for Innovation, Deutsche Forschungsgemeinschaft within CFN

10:36AM A11.00012 Low-temperature transport in highly disordered films of superconducting magnesium diboride . NICHOLAS BREZNAY, AHARON KAPITULNIK, Stanford University — Many features make magnesium diboride an interesting model system for understanding the behavior of two dimensional BCS superconductors, including its sensitivity to disorder and low spin-orbit coupling. We study the transport behavior of highly disordered magnesium diboride films, and will review preliminary low-temperature magnetoresistance measurements in the regime of high magnetic fields. We connect these results to recent work on multilayered films prepared using a similar process and also to similar work on other model systems, and review prospects for future study.

10:48AM A11.00013 $T_c$ vs Isotopic Mass and vs Residual Resistivity Investigation in MgB\textsubscript{2}, MARINA PUTTI, University of Genova, MATTEO TROFEO, PAOLO BROTO, CARLO FERDIGHINI, ENRICO CALLEANI, PIETRO MANFRIETTI, ANDREA PALENZONA — Almost five years after the discovery of superconductivity in MgB\textsubscript{2} the isotope effect on $T_c$ is not yet understood (M. Calandra et al, Physica C456, 38 (2007) and references therein). The isotope effect is mainly due to the B atoms reflecting the important role of B vibrations in determining $T_c$. Detailed two bands calculation leads to $\alpha(B)$ of the order of 0.4–0.45, in disagreement with experiments which evaluated $\alpha(B) = 0.30$. Anharmonicity was proposed as a possible explanation for the reduced B isotope coefficient, but recently it was emphasized that such an explanation needs to be reconsidered. On the other hand, recent investigations on the effect of disorder on $T_c$ pointed out that samples with residual resistivity ($\rho_0$) of few $\mu\Omega\text{cm}$ present $T_c$ variations comparable with the intrinsic variations due to isotopic effect. This calls for new investigations of isotopic effect in samples with controlled amount of disorder. Ultra clean Mg\textsuperscript{10}B\textsubscript{2} and Mg\textsuperscript{11}B\textsubscript{2} samples ($\rho_0 \sim 0.5 \mu\Omega\text{cm}$) were damaged respectively with annealing and neutron irradiation and $T_c$ and resistivity were measured. $T_c$ vs $\rho_0$ plot shows in both cases a linear relationship allowing us to extrapolate $T_c$ ($\rho_0=0$) for both the sample series. $\alpha(B)$ evaluated by these intrinsic $T_c$ values confirms results of previous report and the crucial role of disorder in determining $T_c$ has been proved.
8:00AM A12.00001 Local density of states in Luttinger liquids with a dynamically-generated spin gap, DIRK SCHURICHT, The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK, AKBAR JAEFARI, University of Illinois at Urbana-Champaign, FABIAN ESSELER, The Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We present a theory of STM spectroscopy in semi-infinite 1D strongly correlated electron systems with a spin-gap. We calculate the local density of states of semi-infinite Luttinger liquids with open boundary conditions and a dynamically generated spin gap at zero temperature. In order to perform this calculation, we use the boundary state formalism [1] together with a form factor expansion in the infinite system. We find explicit expressions for the local density of states as a function of the gap size and the distance from the boundary. We show how a local spectroscopic probe of this type can be used to detect the spectrum of fractionalized massive solitons and their dynamics, b) the existence of boundary states and c) charge order induced by the boundary. We will discuss the relevance of this work to STM experiments in 1D systems and in quasi-1D systems used to model stripe phases in strongly correlated systems [2]. [1] S. Ghoshal and A. Zamolodchikov, Int. J. Mod. Phys. 9, 3841(1994), ibid. 9, E4353(1994). [2] S. A. Kivelson, I. P. Bindloss, E. Fradkin, V. Oganesyan, J. Tranquada, A. Kapitulnik and C. Howald, Rev. Mod. Phys. 75, 1201(2003).

8:12AM A12.00002 Spin-Incoherent Luttinger Liquid-Superconductor Hybrid Systems, DAGIM TILAHUN, The University of Texas at Austin, GREGORY FRIEТЕ, California Institute of Technology — Strongly interacting one-dimensional systems exhibit the exotic property of spin-charge separation where a repulsive interaction suppresses the velocity of the spin degree of freedom while enhancing that of the charge. Spin-incoherent Luttinger liquids exist in the regime where the temperature is much higher than the characteristic energy of the spin sector (thermalized, random spins) but much less than that of the charge. We study a hybrid system consisting of a spin-incoherent Luttinger liquid adjoined at one or both ends to a superconductor, and find robust features that can be used as clear experimental signatures of spin-incoherence. We find the tunneling density of states diverges at low energies and exhibits an universal frequency dependence independent of the strength of the interactions in the system. We also find that in spite of exponentially decaying pair correlations with distance into the spin-incoherent Luttinger liquid, the Josephson current remains robust. Compared to the zero temperature Luttinger liquid case there is a factor of 2 reduction in the critical current and a halving of the period in the phase difference between the superconductors. Our results open the way for a new class of experiments in the spin-incoherent regime of one dimensional systems.

8:24AM A12.00003 Temperature dependence of the anomalous exponent in Li(0.9)Mo(6)O(17) that reveals Luttinger Liquid behavior, RENE MATZDORF, TATJANA NOVGORODOV, BERNARD NANSSEU, MICHAEL WAELSLCH, University of Kassel, JIAN HE, RONGYING JIN, DAVID MANDRUS, Oak Ridge National Laboratory — Scanning tunneling spectroscopy (STS) has been used to study the Luttinger-liquid behavior of the purple bronze Li(0.9)Mo(6)O(17) in the temperature range 5K ≤ T ≤ 300K. In the entire temperature range the suppression of density of states at the Fermi-energy could be fitted very well by a model describing the tunneling into a Luttinger liquid at ambient temperature. The power-law extracted from these fits reveals a significant increase above 200K. It changes from α=0.6 at low temperature to α=1.0 at room temperature.

8:36AM A12.00004 Specific heat of a one-dimensional interacting Fermi system, ANDREY CHUBUKOV, University of Wisconsin, DMITTR MASLOV, University of Florida, RONJOY SAHA, University of Oregon — We re-visit the issue of the temperature dependence of the specific heat C(T) for interacting fermions in 1D. The charge component C_{c}(T) scales linearly with T, but the spin component C_{s}(T) displays a more complex behavior with T as it depends on the backscattering amplitude which falls down under RG transformation and eventually behaves as \( g_{s}(T) \sim 1/ \log T \). We show, however, by direct perturbative calculations that C_{s}(T) is strictly linear in T to order \( g_{s}^{2} \) as it contains the renormalized backscattering amplitude not on the scale of T, but at the cutoff scale set by the momentum dependence of the interaction around 2k_{F}. The running amplitude \( g_{s}(T) \) appears only at third order and gives rise to an extra \( T \log^{3} T \) term in C_{s}(T). This agrees with the results obtained by a variety of bosonization techniques. We also show how to obtain the same expansion in \( g_{s} \) within the sine-Gordon model.

8:48AM A12.00005 Entanglement and quantum phase transition in the ground state of one-dimensional asymmetric Hubbard model, WENLING CHAN, SHI-JIAN GU, Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Hong Kong, China — We study the quantum phase transition by means of entanglement in the ground state of the one-dimensional asymmetric Hubbard model. Both the half-filling and away from half-filling cases are investigated. The local entanglement between the middle two sites with the rest of the system, and the block entanglement between the left and right portions of the system, are calculated by the DMRG method. We find that the entanglements show interesting scaling and singular behavior around the phase transition line.

9:00AM A12.00006 Is the Drude weight a thermodynamic quantity?, MARCOS RIGOL, B. SRIRAM SHASHTRY, University of California, Santa Cruz — Transport properties distinguish metals from insulators, and superconductors from ideal metals. In one dimension, they can help differentiate integrable from nonintegrable systems. The Drude weight (or charge stiffness) is found to be nonzero in integrable metals, even at very large temperature, whereas it vanishes for generic (nonintegrable) systems. In systems with periodic boundary conditions, the Drude weight can be shown to be identically zero for any finite system, regardless of its integrability. For the Drude weight to be a thermodynamically meaningful quantity, both kinds of boundary conditions should produce the same answer in the thermodynamic limit. We resolve this paradox using analytical and numerical methods.

9:12AM A12.00007 Phase diagram of hole doped two-leg Cu-O ladders, PIOTR CHUDZINSKI, MARC GABAY, Laboratoire de Physique des Solides, Bat. 510, Université Paris-Sud 11, Centre d’Orsay, 91405 Orsay Cedex, France, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland — In the weak coupling limit, we establish the phase diagram of a two-leg ladder with a unit cell containing both Cu and O atoms, as a function of doping. We use bosonization and design a specific RG procedure to handle the additional degrees of freedom. Significant differences are found with the single orbital case; for purely repulsive interactions, a completely massless quantum critical region is obtained at intermediate carrier concentrations (well inside the bands). For some finite value of direct hopping between oxygen atoms the ground state consists of an incommensurate pattern of orbital currents plus a spin or charge density wave (DW) structure. The experimental relevance of these findings is also discussed. We have calculated the NMR properties like Knight shift and relaxation rate at each atom inside the elementary cell. We make a prediction that different temperature dependance indicates the phase of the measured system.

9:24AM A12.00008 Groundstate fidelity and the spin one chain, IAN MCCULLOCH, University of Queensland — it has been recognized quite recently that the groundstate fidelity, that is, the overlap of the groundstate wavefunctions as a function of interaction strength, can be used to obtain phase boundaries and exponents without a-priori knowledge of the order parameter. This procedure is easy to apply in a wide class of numerical algorithms based on matrix product states, of which the Density Matrix Renormalization Group (DMRG) is the most famous. I will give a brief overview of the technique, and demonstrate that the fidelity reveals all features of the bilinear-biquadratic spin one chain, while almost certainly ruling out the appearance of a (gapped or critical) nematic phase in the vicinity of \( \theta = -3\pi/4 \).
9:36AM A12.00009 Magnetism of one-dimensional Wigner lattices and its impact on charge order. MARIA DAGHOFER, Univ. of Tennessee, Knoxville, REINHARD NOACK, Philips Universitaet Marburg, PETER HORSCHE, MPI for Solid State Research, Stuttgart — We report the phase diagram of a quarter-filled Wigner lattice described by the 1D Hubbard-Wigner model with nearest and next-nearest neighbor hopping $t_1$ and $t_2$. In the $t_1$-$t_2$ plane, we find a region at negative $t_2$ with fully saturated ferromagnetic ground states due to kinetic exchange interactions, while the remaining phase diagram is controlled by antiferromagnetic exchange. We also observe a strong influence of magnetism on the charge structure factor, in contrast to the expectation that charge ordering in the Wigner lattice is well described by spinless fermions. Our results, obtained using the density-matrix renormalization group and exact diagonalization, can be transparently explained within the framework of an effective low-energy Hamiltonian.

9:48AM A12.00010 Critical lines and massive phases in quantum spin ladders with dimerization. JAVIER ALMEIDA, MIGUEL ANGELO MATIN-DELGADO, Universidad Complutense, Madrid, Spain, GERMAN SIERRA, Instituto de Fisica Teorica, C.S.I.C-U.A.M, Madrid, Spain — We study here various types of $S=1/2$ spin ladders with odd and even number of legs and intrinsically dimerized patterns. The low temperature physics of these systems is very rich and in fact their ground state at $T=0$ may undergo a quantum phase transition as we vary the microscopic parameters of the lattices. To study these many-body systems we will use the density matrix renormalization group (DMRG) algorithm, and will present accurate estimations of the critical lines found in these models as well as different measurements to characterize the nature of the ground state. We will see that the valence bond solid picture seems to be a proper description of the massive phases on each side of the phase diagram and will show evidences of this nature by means of a particular order parameter denoted generalized string order parameter.

10:00AM A12.00011 ABSTRACT WITHDRAWN —

10:12AM A12.00012 Magnetostriction and thermal expansion on 1D chain compound Azurite, FREDDERIK W. FABRIS, VIVIEN ZAPF, SONIA FRANCOUAL, MARCELO JAIME, ALEX LACERDA, National High Magnetic Field Laboratory, Los Alamos, New Mexico 87545, USA, NHMFL-LANL TEAM — Azurite is a natural mineral with a chemical structure Cu$_3$(OH)$_2$(CO$_3$)$_2$. This compound is a frustrated triangular quantum magnet consisting of Cu S=1/2 atoms arranged alternately to form infinite chains along the b axis. The magnetic behavior of this compound reflects the existence of both monomers and dimers of $S=1/2$ Cu. A magnetization plateau at 1/3 of the saturation magnetization is observed in M vs H measurements between 11 and 30 T due to saturation of the monomers. For fields above the plateau, the magnetic field energy exceeds the dimer bonding and thus the dimers cant and then align with the field. The magnetic structure and the detailed phase diagram in temperature and field are largely unknown or controversial. A recent report [1] in the specific heat behavior suggests a more complicated structure than previously thought. In addition, recent ultrasound measurements [2] indicate significant magnetoelastic coupling must be taken into account. We have acquired interesting results on magnetic torque, magnetostriction and thermal expansion. We have demonstrated that significant, anisotropic magnetostriction occurs in azurite, giving us an indication of the magnetically induced structural distortions. [1] Yasu Takeho, personal communication. [2] Lang et al, J. Phys.: Conf. Series 51, 1. (2006).

10:24AM A12.00013 Quantum Monte Carlo study of a spin-Peierls model in a magnetic field1, JEONGPIL SONG, R.T. CLAY, Mississippi State University — We present results of a quantum Monte Carlo study of a quasi one-dimensional XY spin model coupled to quantum phonons. We compare different updating techniques for the Stochastic Series Expansion method and present autocorrelation time data. We are able to reduce autocorrelation times by using loop update techniques for both spin and phonon degrees of freedom. We determine the critical phonon coupling for the spin-Peierls state, and discuss the dependence on the phonon frequency, magnetic field, and inter-chain coupling.

1Supported by the Department of Energy grant DE-FG02-06ER46315.

10:36AM A12.00014 Quantum solvation in optical lattice, YOU WENLONG1, GU SHIJIAN, LIN HAIQING, Department of Physics, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong, CUHK TEAM — We have studied the ground state phase diagram of the one dimensional asymmetric t-J-2 model at various filling by different methods. The reduced dimensionality and asymmetric hopping could lead to interesting dynamics which can be conjectured to demonstrate quantum solvation process with fermion character of the quantum solvent. The system potentially can be demonstrated in optical lattice.

1Department of Physics, Peking University, Beijing 100871, China

10:48AM A12.00015 Effective model parameters for the spin-Peierls system TiOCl from first principles, YUZHONG ZHANG, ROSER VALENTI, HARALD JESCHKE, Johann Wolfgang Goethe-Universität, Institut füer Theoretische Physik — The inorganic spin-Peierls system TiOCl is studied in the frame of Density Functional Theory (DFT) by the projector augmented wave (PAW) and linearized augmented plane wave (LAPW) methods. A two-dimensional frustrated spin Peierls model is proposed to describe the system. The model parameters, such as spin exchange couplings in a, b, and c directions, are estimated by the LAPW method. With the help of the eigenvectors of the dynamical matrix, the spin-phonon couplings and the elastic constant are determined by the PAW method. The reliability of these model parameters is demonstrated by an exact diagonalization and a mean-field calculation as well as by comparison to available experiments.

Monday, March 10, 2008 8:00AM - 10:36AM –
Session A13 DCOMP GSCCM: Focus Session: Simulations of Matter at Extreme Conditions I: Hydrogen Helium, and Planetary Materials

8:00AM A13.00001 Quantum Monte Carlo Simulations of Warm Dense Hydrogen1, DAVID CEPERLEY, University of Illinois Urbana-Champaign — Quantum Monte Carlo methods are the most accurate and general methods for computing total electronic energies. However, in general, they have been limited to the temperatures or to zero temperature. In recent years, we and others have been working on methods [1] that utilize the Born Oppenheimer approximation to allow simulations coupling the correlated quantum systems and a system of ions. Using quantum Monte Carlo, one estimates the Born-Oppenheimer energy change for a movement of the ions which is then used in a Monte Carlo simulation of the ionic degrees of freedom. The quantum effects of the ionic degrees of freedom and the boundary conditions on the phase of the wavefunction can be integrated over. We have performed simulations of dense hydrogen down to temperatures of 300K. We have used this method to determine the equation of state of warm dense hydrogen, to study the cross-over from the molecular liquid to the atomic liquid [2] and for the melting temperature of solid atomic hydrogen [3].


1DOE DE-FG52-06NA26170 and computer resources from INCITE and NCSA.
8:36AM A13.00002 Electrical conductivity of liquid Hydrogen
1. FEI LIN, University of Illinois at Urbana-Champaign, KRIS DELANEY, University of California, Santa Barbara, MIGUEL MORALES, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, University of L’Aquila, RICHARD MARTIN, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — DC electrical conductivity of liquid Hydrogen under high pressure has been measured by shock-wave experiments a long time ago [Phys. Rev. Lett. 76, 1860 (1996)], however, an accurate theoretical calculation of electrical conductivity is still unavailable. Ab-initio DFT calculations seem to overestimate the DC conductivity value by about 6 times. On the other hand, coupled electron-ion—Quantum Monte Carlo (CEIMC) simulation [Phys. Rev. Lett. 97, 235702 (2006)] has predicted different high-pressure Hydrogen molecular-atomic transition than the DFT calculation. In this talk I will report our preliminary electrical conductivity results from CEIMC simulations using the Kubo formula with energies and current-current matrix elements computed with correlated quantum Monte Carlo methods.

1Supported by DE-FG52-06NA26170 and computer resources of NCSA.

8:48AM A13.00003 Properties of Hydrogen-Helium Mixtures at High Pressure and Temperature
1. SAAD KHAIRALLAH, Earth and Planetary Science Department, University of California, Berkeley, JAN VORBERGER, Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom., BURKHARD MILITZER, Earth and Planetary Science Department, University of California, Berkeley. — Most of the over 200 recently discovered extrasolar planets are giant gas planets that consist primarily of dense, hot hydrogen and helium. Using density functional molecular dynamics (DFT-MD) simulations, we study these fluids at the extreme conditions found in planet interiors. We characterize the interaction of hydrogen and helium, analyze the electronic properties, and report on structural changes in the fluid as a function of density and temperature. We further study the influence of helium concentrations on the stability of hydrogen molecules.

1NASA grant PGG04-0000-0116, NSF grant 0507321.

9:00AM A13.00004 Ultra-High-Pressure Water. MARTIN FRENCH, RONALD REDMER, Universitat Rostock, Institut fur Physik, D-18051 Rostock, Germany, THOMAS R. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185-1186, USA. — We present the first all-electron QMD simulations of water in the ultra-high-pressure regime up to conditions typical for the deep interior of Jupiter and Saturn. We calculate the equation of state and the Hugoniot curve and study the structural properties via pair correlation functions and self-diffusion coefficients. In the ultra-dense superionic phase, we find a continuous transition in the protonic structure. Water at conditions of Jupiter’s core (i.e. 20000 K, 50 Mbar, 11 g/cm^3) forms a fluid dense plasma. Supported by the DFG within SFB 652. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:12AM A13.00005 Ab initio Molecular Dynamics Simulations of Water Under Shock Compression: Chemistry Behind Shock Fronts. LAURENCE FRIED, NIR GOLDMAN, Lawrence Livermore National Laboratory, ALESSANDRO CURIONI, IBM Research, Zurich Research Laboratory, CHRISTOPHER MUNDY, Pacific Northwest National Laboratory, I.-F.W. KUO, EVAN REED, Lawrence Livermore National Laboratory — We report herein first principles simulations of water under shock loading of velocities from 5 - 11 km/s. Accurate description of the plateau in the ionic conductivity at high pressures and temperatures is of particular importance to models of the planetary dynamo mechanism in Neptune and Uranus. We attribute this plateau to the exceedingly short-lived molecular and ionic states that occur in water under these extreme conditions. In particular, at the intersection of the shock hugoniot and Neptune isentrope we observe transient metalization that we attribute to the formation of short-lived negatively charged species that contribute electronic states at or around the band gap.

9:24AM A13.00006 Molecular structures of CO2 and N2O under pressure1. STANIMIR A. BONEV, BRENDAN OSBERG, Department of Physics, Dalhousie University, Canada — Carbon dioxide and nitrous oxide are investigated at pressures up to 50 GPa and 1000 K using ab initio methods. In this pressure-temperature range, both materials have a number of stable molecular structures. We demonstrate that the constituent molecules in these structures do not undergo significant changes and that the proposed phases are consistent with experimental data. The differences found between the CO2 and N2O phase diagrams can be understood in terms of the polarity of the N2O molecules.

1Work supported by NSERC.

9:36AM A13.00007 Quantum Monte Carlo Computations for Equations of State, Phase Transitions, and Elasticity of Silica, R.E. COHEN, Carnegie Institution of Washington, B. MILITZER, Z. WU, University of California, Berkeley, K. DRIVER, Ohio State University, P.L. RIOS, M. TOWLER, R. NEEDS, University of Cambridge — We have performed Quantum Monte Carlo (QMC) computations for silica in the quartz, stishovite, and α-PbO2 structures as functions of compression. In spite of the great success of DFT there is still need for improvement. The local density approximation (LDA) gives excellent results for individual silica phases, but LDA predicts stishovite to be the stable ground state rather than quartz. The Generalized Gradient Approximation (GGA) does give correct energy differences, but other properties, such as the bulk moduli, are worse with the GGA than the LDA. We included thermal contributions using density functional perturbation theory with the code ABINIT. We have also computed the shear elastic constant c21-c22 in stishovite, which is associated with the phase transition to the CaCl2 structure, with QMC. We find excellent agreement with experiments. We find that the main differences found between QMC and DFT are crystalline phase dependent energy and pressure shifts. This work is supported by NSF grants EAR-0530282, EAR-0310139, and by DOE contract DE-FG02-99ER45795 to John Wilkins. Computations were performed on blueice at NCAR under a BTS grant, and on Tungsten and Abe at NCSA, and at the Carnegie Institution of Washington.

9:48AM A13.00008 The effect of temperature and anisotropic pressure on the phase transitions in α-cristobalite. ROMAN MARTONAK, Comenius University, SK., DAVIDE DONADIO, UC Davis, PAOLO RAITERI, MICHELE PARRINELLO, ETH Zurich, CH — The role of temperature and anisotropy of the pressure tensor in the pressure-induced transformations of α-cristobalite is investigated by means of first principle molecular dynamics combined with an improved version of the metadynamics algorithm for the study of solid-solid phase transitions. We reproduce for the first time the transition to α-PbO2 as found in experiment[4] and we observe that the transition paths are qualitatively different and yield different products whether the applied pressure is hydrostatic or not. While in hydrostatic conditions α-PbO2 or stishovite is obtained depending on the temperature and initial conditions, more complicated pathways with several metastable structures are followed upon non-hydrostatic compression and post-stishovite phases are obtained. Based of our simulations, we predict the metastability of a new class of high pressure polymorphs of silica obtained by non-hydrostatic compression.

The inter-vortex distance is given by \( \theta = \frac{\pi}{2 \pi l} \approx \frac{805 \text{ nm}}{8 \pi l} \), where \( l \) is the condensate diameter, and \( \phi \) is the optical wavelength. We prepare the condensate in the dressed state, whose projection onto internal states of various state-dependent Bragg momenta are well understood.

The results may bring important implications to interior models of giant planets, which may lead to a better understanding in giant planets physics.

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A14 GQI DAMOP: Focus Session: Quantum Simulation of Condensed Matter Systems With Ultracold Atoms
Morial Convention Center 205

8:00AM A14.00001 Simulating Charged Particles in a Magnetic Field with Ultra-cold Atoms Using Light-induced Effective Gauge Fields, YU-JU LIN, WILLIAM PHILLIPS, JAMES PORTO, IAN SPIELMAN, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY TEAM, UNIVERSITY OF MARYLAND TEAM — We experimentally study light-induced gauge potentials in a \(^{87}\)Rb Bose-Einstein condensate. Instead of rotating the trap, we prepare the atoms in a spatially-varying optically dressed state. The atomic spin state is dressed by a spatially varying two-photon Raman coupling between the three \( F = 1 \) hyperfine ground states. The resulting effective magnetic field is equivalent to rotating the condensate (and transforming to the rotating frame), and thus generates vortices. The inter-vortex distance is given by \( \theta = \frac{\pi}{2 \pi l} \approx \frac{805 \text{ nm}}{8 \pi l} \), where \( l \) is the condensate diameter, and \( \phi \) is the optical wavelength. We prepare the condensate in the dressed state, whose projection onto internal states of various state-dependent Bragg momenta are well understood.

8:12AM A14.00002 Two-Dimensional Electron Gas with Cold Atoms in Non-Abelian Gauge Potentials, INDUBALA SATIJA, Department of Physics, George Mason University, DANIEL DAKIN, Optical Air Data Systems, J. Y. VAISHNAV, CHARLES W. CLARK, Joint Quantum Institute, National Institute of Standards and Technology — Motivated by the possibility of creating non-Abelian fields using cold atoms in optical lattices, we study two-dimensional electron gases in a lattice, subjected to such fields. In the continuum limit, the system characterized by a two-component “magnetic flux” describes a harmonic oscillator existing in two different charge states (mimicking a particle-hole pair). A key feature of the non-Abelian system is a splitting of the Landau energy levels, which broaden into bands. These Landau bands result in a coarse-grained Hofstadter “moth.” Furthermore, the bands overlap, leading to effective relativistic effects. Similar features also characterize the corresponding 2D lattice problem when at least one of the components of the magnetic flux is an irrational number. Some unique aspects of the transport properties of the non-Abelian system are the possibility of inducing localization by varying the quasimomentum, and the absence of localization of certain zero-energy states exhibiting a linear dispersion relation. Furthermore, non-Abelian systems provide an interesting localization scenario where the localization transition is accompanied by a transition from relativistic to non-relativistic theory.

8:24AM A14.00003 Observing Zitterbewegung in Ultracold Atoms, J.Y. VAISHNAV, CHARLES W. CLARK, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg MD 20899 — We propose an optical lattice scheme which would permit the experimental observation of Zitterbewegung (ZB) with ultracold, neutral atoms. A four-level “tripod” variant of the usual setup for stimulated Raman adiabatic passage (STIRAP) has been proposed for generating non-Abelian gauge fields. [1] Dirac-like Hamiltonians, which exhibit ZB, are simple examples of such non-Abelian gauge fields; we show how a variety of them can arise, and how ZB can be observed, in a tripod system. We predict that the ZB should occur at experimentally accessible frequencies and amplitudes.


8:36AM A14.00004 Detecting the Bose glass in optical lattices, TOMMASO ROSCILDE, Max-Planck Institute for Quantum Optics — We theoretically propose a method for the unambiguous experimental detection of Bose-glass behavior in the central region of a system of bosons trapped in an optical lattice system, and to discriminate the Bose glass from more conventional Mott and band insulators. The method is based on probing the compressibility of the system in the trap center by gradually increasing the trap frequency. Straightforward measurements of the average particle density in the center of the trap and of the momentum distribution allow to detect the migration of particles from the wings into localized states in the center of the system under trap squeezing. We discuss the application of the method to simple optical lattices, and to commensurate and incommensurate optical superlattices; we moreover discuss the potential of trap squeezing techniques to probe the density of states of exotic phases realized in optical lattices.
8:48AM A14.00005 Phase Coherence and Superfluid-Insulator Transition in a Disordered Bose-Einstein Condensate. YONG P. CHEN, J. HITCHCOCK, D. DRIES, M. JUNGER, C. WELFORD, R. G. HULET, Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston TX 77005 USA — We have studied both the transport and phase coherence properties of a Bose-Einstein condensate (BEC) of $^7$Li atoms subject to a disordered potential with tunable strength ($V_D$). The BEC is created in an elongated optical trap, while the disordered potential is produced by laser speckle. We probe transport of the disordered BEC by either slowly or abruptly offsetting the trap relative to the disordered potential. At high $V_D$, we observe pinning of the disordered BEC and suppression of its dipole excitation, consistent with the transition to an insulator. We use in-situ imaging to detect density modulation, while time-of-flight (TOF) imaging is used to probe phase coherence. At moderate $V_D$, we observe small density fluctuations in the in-situ images, and random but reproducible interference patterns in the TOF images. This interference reflects phase coherence in the disordered BEC and is interpreted as speckle for matter waves. At higher $V_D$, the TOF interference contrast diminishes while the in-situ density fluctuations increase, signifying a fragmented “granular” condensate with little phase coherence. 1Supported by NSF, ONR, NASA, Welch and Keck Foundations. 2Now at Purdue University.

9:00AM A14.00006 Effects of disorder on the interacting Fermi gases in one-dimensional optical lattices. B. TANATAR, Physics Department, Bilkent University, 06800 Ankara, Turkey, GAO XIANLONG, Physics Department, Zhejiang Normal University, Jinhua, 321004 China, M. POLINI, M. P. TOSI, NEST-CNR-INFM and Scuola Normale Superiore I-56126 Pisa, Italy — Interacting two-component Fermi gases loaded in a one-dimensional (1D) lattice and subjected to a harmonic trapping potential exhibit interesting compound phases in which fluid regions coexist with local Mott-insulator and/or band-insulator regions. Motivated by experiments on cold atoms inside disordered optical lattices, we present a theoretical study of the effects of a random potential on these ground-state phases. We employ density-functional theory within the local-density approximation to determine the density distribution of fermions in these phases. The exchange-correlation potential is obtained from the Lieb-Wu exact solution of Fermi-Hubbard model. On-site disorder and harmonic trap are treated as external potentials. We find that disorder has two main effects: it destroys the local insulating regions if it is sufficiently strong compared with the on-site atom-atom repulsion, and it induces an anomaly in the compressibility at low density from quenching of percolation.

9:12AM A14.00007 Probing non-local order parameters in highly correlated Bose insulators. EHUD ALTMAN, Department of Condensed Matter Physics, Weizmann Institute of Science — Ground states of integer spin chains are known since the late 80’s to sustain highly non-local order described by infinite string operators of the spins. Such states defy the usual Landau theory description and can be considered simple prototypes of topological order. Recently we showed that spinless Bose insulators with nearest neighbor or longer range repulsion in one dimension can exhibit similar string order in terms of the boson density [1]. The tunability of cold atomic systems would allow much more flexibility in probing the non-local order than spin systems do. For example the bosons can be tuned across a quantum phase transition between the exotic insulator, which we term Haldane insulator, and the usual Mott insulator. Investigating how the transition responds to external perturbations lends direct access to properties of the string order parameter. I will demonstrate this with several new results obtained from a field theoretic description of the phases and confirmed by numerical calculations using DMRG. Particularly revealing of the unusual character of the string order is the prediction that any external perturbation, which breaks the lattice inversion symmetry, would eliminate the distinction between the Haldane and Mott phases and allow a fully gapped adiabatic connection between them. This is remarkable given that neither phase involves spontaneous breaking of lattice inversion symmetry. We also predict that inter-chain tunneling destroys the direct phase transition between the two insulators by establishing an intermediate superfluid phase. Finally I will discuss how the new phases and phase transitions may be realized and probed in actual experiments with ultra cold atoms or polar molecules.

9:48AM A14.00008 A Hexagonal Lattice Ion Trap for Quantum Simulation of Spin Models. ZILIANG LIN, ROBERT CLARK, YUEFEI GE, ISAAC CHUANG, Massachusetts Institute of Technology. PLANAR LATTICE TRAP TEAM — Quantum simulations of one dimensional spin systems are being implemented by ions in linear Paul traps; however, a natural extension to two dimensional quantum spin simulations cannot be realized in the linear Paul trap geometry. Planar lattice traps not only offer the possibility for two dimensional simulations, but also hold two advantages over linear traps: first, neighboring ions in lattice traps have well defined and uniform spacings; second, quantum simulations with planar traps may be scaled up more easily than with linear traps. We develop a hexagonal lattice trap that allows vibrational coupling between ions due to their Coulomb repulsion, which is essential for effective spin-spin interaction. We present fabrication details, preliminary testing results, and a proposal for simulating geometrical spin frustration with three ions in a triangular configuration.

10:00AM A14.00009 Trapped-Ion Quantum Simulations of Spin Systems: From Two Qubits to Thousands. WARREN LYBARGER, Los Alamos National Laboratory, DANA BERKELAND, IARPA, JOHN CHIAVERINI, Los Alamos National Laboratory — Due to the exponential growth of a quantum system’s state-space with its size, the current technological limit for simulating the evolution of many-qubit spin systems with classical computers (CC) is 36 spin-$\frac{1}{2}$ particles. While CC’s cannot be scaled to meet the exponentially increased demand in computational resources, mapping the Hamiltonians of such problems onto that of a quantum simulator (QS) completely avoids this exponential scaling problem, allowing for efficient simulations of much larger systems. QS may be the first attainable application of quantum information processing, enabling exploration of parts of the phase space not accessible in the original system and possibly providing an exponential speedup of computations for even just a few tens of interacting qubits when compared to CC methods. Following the work of Porras and Cirac [Phys. Rev. Lett. 92. 207901-1 (2004)] we discuss the status of an experiment at Los Alamos for demonstrating a proof of principle QS of an Ising-like spin-spin interaction in a transverse magnetic field. We also discuss a novel architecture for microfabricated ion trap arrays geared toward enabling large scale QS and one-way quantum computing with potentially thousands of ions [arXiv:0711.0233].

10:12AM A14.00010 Quantitative determination of the Hubbard model phase diagram from optical lattice experiments: overcoming the singular nature of the thermodynamic limit. VIVALDO CAMPO, JR., Unidade de Brasilia, Brazil and Universidade de Sao Paulo, Brazil, KLAUS CAPELLE, Universidade de Sao Paulo, Brazil, JORGE QUIN- TANILLA, Rutherford Appleton Laboratory, U.K., CHRIS HOOLEY, University of St Andrews, U.K. — We propose an experiment to obtain the phase diagram of the fermionic Hubbard model, for any dimensionality, using cold atoms in optical lattices. It is based on measuring the total energy for a sequence of trap profiles. It combines finite-size scaling with an additional ‘finite-curvature scaling’ necessary to reach the homogeneous limit. We illustrate its viability in the 1D case, simulating experimental data in the Bethe-Ansatz local density approximation. Including experimental errors, the filling corresponding to the Mott transition can be determined with better than 3 per cent accuracy. The main obstacle that our method overcomes is the singular nature of the thermodynamic limit of atom traps. We discuss this surprising phenomenon and describe a simpler experiment that could be used to demonstrate it.
10:24AM A14.00011 The p$_{x,y}$-orbital counterpart of graphene – cold fermions in the honeycomb optical lattices, CONGJUN WU, Physics Department, UCSD, DORON BERGMAN, Physics Department, Yale, LEON BALENTS, Physics Department, UCSB, SANKAR DAS SARMA, Physics Department, Univ. of Maryland — We study the ground states of cold atoms in the tight-binding bands built from p-orbitals on a two dimensional honeycomb optical lattice. The band structure includes two completely flat bands. Exact many-body ground states with on-site repulsion can be found at low particle densities, for both fermions and bosons. We find crystalline order at $n=1/6$ with a $\sqrt{3} \times \sqrt{3}$ structure breaking a number of discrete lattice symmetries. In fermionic systems, if the repulsion is strong enough, we find the bonding strength becomes dimerized at $n=1/2$. Experimental signatures of crystalline order can be detected through the noise correlations in time of flight experiments.

10:36AM A14.00012 DMRG Studies for Strongly-Correlated Fermions on a Triangular Optical Lattice, MASAKI OKUMURA, SUSUMU YAMADA, MASAKI MACHIDA, CCSE, Japan Atomic Energy Agency and JST(CREST) — Strongly-interacting fermions in a triangular lattice attract much attention because not only the interaction but also the geometrical frustration is expected to cause non-trivial behaviors. In solids, most of materials parameters, e.g., interaction strength between electrons (fermions), fermion density, and crystalline potential are almost fixed depending on the sample and our research area are restricted. In contrast, cold atom systems enable to study it systematically because some crucial parameters are precisely controllable. Thus, we expect that the cold Fermi atoms on a triangular lattice bring us information on both strongly-correlated and frustrated systems. In this study, we examine a system described by the triangular Hubbard model by using the parallel density-matrix renormalization group (DMRG). In addition, we also investigate effects of random potential made by speckle laser in the system. We evaluate the effects of frustration, strong interaction, and randomness simultaneously.

10:48AM A14.00013 Order parameter statistics at a quantum phase transition, AUSTEN LAMACRAFT, University of Virginia, PAUL FENDLEY, University of Virginia and All Souls College, Oxford — Universality implies that at a second order phase transition the probability distribution of the order parameter takes a universal scaling form. This distribution is a natural way to characterize the quantum critical properties of ultracold atomic gases, since its histogram may be readily obtained by repeated 'single-shot' measurements. In this work we obtain the exact scaling probability distribution for the simplest quantum critical point: that of the transverse field Ising model in 1D. Using a novel identity for the Ising model correlation functions, we map the problem to a particular case of the anisotropic Kondo model.

Monday, March 10, 2008 8:00AM — 10:48AM — Convention Center 207

8:00AM A15.00001 Bias dependence of magnetic exchange coupling, PAUL HANEY, MARK STILES, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, CHRISTIAN HEILIGER, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Maryland NanoCenter, University of Maryland, ALLAN MACDONALD, The University of Texas at Austin — An applied electrical bias can change the interlayer coupling in magnetic multilayers and magnetic tunnel junctions. The bias dependence of these changes is ultrafast; it is not clear whether the changes depend linearly or quadratically on the applied voltage. Motivated by this controversy, as well as proposals to exploit bias-dependent exchange coupling to accomplish current induced magnetic switching, we compute the bias-dependence of interlayer exchange coupling in magnetic multilayers and tunnel junctions. For simple tight-binding models, we derive expressions for this dependence, describe the special cases in which this dependence is particularly large, and derive the extent to which zero-bias expressions for interlayer coupling remain valid for biased systems. We also examine the related question of the bias-dependence of intralayer exchange interactions in a single ferromagnetic layer, and discuss experimental consequences of bias-modulated exchange stiffness, including induced changes in the Curie temperature and spin wave dispersion. This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement.

8:12AM A15.00002 Spin current and rectification in quantum wires, FEIFEI LI, Department of Physics, Brown University, Providence, Rhode Island 02912 USA, BERND BRAUNECKER, Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, DIMA FELDMAN, Department of Physics, Brown University, Providence, Rhode Island 02912, USA — We study the spin and charge currents in a one-channel quantum wire with strong electron interactions in a uniform static magnetic field. We show that a dc-spin current can be generated by an ac voltage in the presence of an asymmetric potential barrier, e.g., two point scatterers of unequal strength. In an interval of voltages, the spin current increases with the decrease of the voltage bias as a negative power of the voltage. We find that the spin dc-current in units of electron charge per second can greatly exceed the charge current in units of electron charge per second. Neither spin-polarized particle injection nor time-dependent magnetic fields are required for the generation of the spin current.


3This research was supported by NSF under Grant No. DMR-0544116.

8:24AM A15.00003 Vortices and Antivortices as Harmonic Oscillators, B. KRUEGER, M. BOLTE, A. DREWS, U. MERKT, G. MEIER, D. PFANNKUHCE, University of Hamburg, Germany — In experiments the distinction between current-induced dynamics and the dynamics induced by the Oersted field of the current is still an open problem. Here we investigate the gyrosopic motion of current- and field-driven magnetic vortices/antivortices in micro- or nanostructured thin-film elements by analytical calculations and by numerical simulations. Starting from the micromagnetic equation of motion extended by the spin torque introduced by Zhang and Li, we derive an analytical expression for the current- and field-driven trajectory of the vortex/antivortex. The gyrosopic motion is well described by modeling the stray-field energy as a harmonic-oscillator potential. For small harmonic excitations the vortex/antivortex cores perform an elliptical rotation around their equilibrium positions. Our analytical model allows to calculate the amplitude and phase of the gyration. The phase of the rotation and the ratio between semi-axes are determined by the frequency and amplitudes of Oersted field and spin torque. The analytical result is compared to micromagnetic simulations with good accordance.[1] Even though the influence of weak magnetic fields on the vortex/antivortex trajectories is small, the phase of the rotation is significantly changed. Thus, the model can estimate the Oersted field’s contribution in spin-torque experiments.[1] B. Krueger et al., Phys. Rev. B 76, December (2007).

8:36AM A15.00004 Current-induced torques in magnetic textures and in antiferromagnets, REMBERT DUINE, Utrecht University — Current-induced torques on ferromagnetic nanoparticle and on domain walls in ferromagnetic nanowires are normally understood in terms of transfer of conserved spin angular momentum between spin-polarized currents and the magnetic condensate. Spin pumping is the opposite of spin transfer, namely the generation of spin currents by a time-dependent magnetization. In this talk I will discuss recent theoretical work aimed at understanding current-induced torques and spin pumping in situations that spin is not fully conserved, due to e.g., spin-orbit interactions, or when conservation of spin can not be used to infer order-parameter dynamics, as is the case in antiferromagnets.
9:12AM A15.00005 Spin transfer and the role of spin-motive-forces for spin valves and domain walls. STEWART BARNES, Physics Dept., Univ. of Miami — The interaction of magnetic domains with electrical currents has potentially far reaching applications for spintronics. The requirements of energy conservation are reflected by spin- (smf) and electro-motive-forces (emf) [1]. For spin-valves and domain walls this smf redistributes the currents between the different possible conduction channels in a manner that significantly modifies the dynamics and introduces magnetic relaxation. Our Berry phase approach to domain walls [1,2] has been extended to spin-valves. The results are consistent with the requirements of angular momentum and energy conservation but differ in a number of important ways from those obtained when the Stoner-Esaki torque transfer term is added to the Landau-Lifshitz equations with either Gilbert or Landau-Lifshitz relaxation [3].

1 A collaboration with J. Ieda and S. Maekawa.

9:24AM A15.00006 Dynamic and temperature effects in spin-transfer switching. HUY PHAM, University of New Orleans, ALEXANDRU STANCU, Iasi University, LEONARD SPINU, University of New Orleans — Recently, the current-induced spin-transfer torque has been proposed as a convenient writing process in high density magnetic random access memory. With increasing demand on the access time, the current pulse shape become important. Also, with memory area density increasing and the memory cell size further shrinking the study of thermal fluctuations in these magnetic structures becomes of extreme importance for their recording thermal stability. In this paper we have studied the dynamic switching process in spin valves and domain walls using a combination of spin-flip excitation and orbit excitation. We have observed a surprising and so far largely unexplained degeneracy in this system: when (as is often the case) there are two orbits with the same energy, even if their shapes and sizes are very different, their frequencies turn out to be the same. Although this is easy to show in the highest-symmetry (uniaxial) case, we find it is true far more generally — for any quadratic energy function with arbitrary anisotropy tensor and arbitrary external magnetic field. We have calculated the frequencies for a random selection of anisotropy tensors and magnetic fields, will show examples of asymmetrical orbits, whose frequencies are equal within numerical accuracy ($\approx 10^{-15}$).

1 Work supported by DARPA Grant No. HR0011-07-1-0031.

9:36AM A15.00007 Frequency degeneracy in spin-torque induced precession. SHUXIA WANG, PIETER VISSCHER, University of Alabama — Magnetic precession in nanometer elements, first studied by Stoner and Wohlfarth in 1948, is central to the understanding of fast switching in magnetic information storage devices. Periodic orbits have recently gained more attention because they can be stabilized (and their frequencies measured) by spin torque techniques. We have observed a surprising and so far largely unexplained degeneracy in this system: when (as is often the case) there are two orbits with the same energy, even if their shapes and sizes are very different, their frequencies turn out to be the same. Although this is easy to show in the highest-symmetry (uniaxial) case, we find it is true far more generally — for any quadratic energy function with arbitrary anisotropy tensor and arbitrary external magnetic field. We have calculated the frequencies for a random selection of anisotropy tensors and magnetic fields, will show examples of asymmetrical orbits, whose frequencies are equal within numerical accuracy ($\approx 10^{-15}$).


10:00AM A15.00009 Evaluation of Gilbert damping in transition metals using tight binding schemes. CHUNSHENG LIU, CLAUDIA K.A. MEWES, MAIRBEK CHSHIEV, TIM MEWES, WILLIAM H. BUTLER, Center for Materials for Information Technology, The University of Alabama, Tuscaloosa, AL — Recently first principle calculations of the damping in transition metals have reproduced the unusual temperature dependence observed experimentally [1, 2]. Here we present an alternative method to calculate the Gilbert damping within Kamburský’s spin torque correlation model using a combination of first principle calculations and an extended Hückel tight binding model. In our scheme we use ab initio calculations (VASP) including spin orbit coupling to obtain the band structure of the transition metal of interest. With the knowledge of the band structure we use a fitting procedure to construct an extended Hückel tight binding model which then allows the evaluation of the Gilbert damping parameter. Because of the simplicity of our Hamiltonian, we can converge the integral over the Brillouin of the spin-orbit tensor without extraordinary computational effort. We show that our results are in good agreement with the results obtained from previous calculations. [1] K. Gilmore, Y.U. Idzerda and M.D. Stiles, Phys. Rev. Lett. 99, 027204 (2007). [2] V. Kamberský, Phys. Rev. B 76, 134416 (2007).

10:12AM A15.00010 Saturation of spin-polarized current in nanometer scale aluminum grains. CHRIS MALEC, YAGUANG WEI, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — We describe measurements of spin-polarized tunnelling via discrete energy levels of single Aluminium grains. In high resistance samples ($\ll \xi_0$), spin-polarized current is carried only via the ground state and the low-lying excited states, leading to a saturation in spin polarized current with bias voltage. Both a qualitative argument based on relaxation rates, and a non-equilibrium transport model are developed and compared. In two samples, the spin-relaxation rate $T_{1}^{-1}$ for some of the low-lying excited states is comparable to the electron tunnelling rate: $T_{1}^{-1} \approx 1.5 \cdot 10^{9}$ s$^{-1}$ and $10^{7}$ s$^{-1}$, meaning the spin of an electron confined in a metallic grain is highly stable. The ratio of $T_{1}^{-1}$ to the electron-phonon relaxation rate is in quantitative agreement with the Elliot-Yafet scaling, an evidence that spin-relaxation in Al grains is driven by the spin-orbit interaction.

10:24AM A15.00011 Kondo Resonance in the Presence of Spin-Polarized Currents. YUNONG QI, University of Houston, JIAN-XIN ZHU, Los Alamos National Laboratory, SHUFENG ZHANG, University of Missouri-Columbia, CHIN-SHEN TING, University of Houston — We propose an improved method of the equation of motion approach to study the Kondo problem in spin-dependent non-equilibrium conditions. We found that the previously introduced additional renormalization for non-equilibrium Kondo effects is not required when we use a proper decoupling scheme. Our improved formulation is then applied to address the spin-split Kondo peaks when a spin current injects into a Kondo system. We believe that this work significantly advances our understanding of the non-equilibrium Kondo physics, and our predictions of the Kondo resonance are timely for the application of non-equilibrium spin-related phenomena.
10:36AM A15.00012 Resolution-dependent mechanisms for bimodal switching time distributions in simulated Fe nanopillars\(^1\), S.H. THOMPSON, G. BROWN, P.A. RIKVOLD, Florida State U., M.A. NOVOTNY, Mississippi State U. — Numerical simulations of magnetization reversals of iron nanopillars in off-axis applied fields at different lattice resolutions reveal bimodal distributions in the switching times (first-passage times through 0 of the longitudinal magnetization, \(M_z\)). We show that the mechanisms responsible for these distributions are resolution-dependent. The highest-resolution model, in which the computational cell is smaller than the exchange length, is three-dimensional. Here, the bimodal distribution results from a reversal process in which the pillar sometimes avoids a metastable free-energy well. At medium resolution, the pillar is modeled as a 1-D stack of spins. The bimodal distribution then reflects whether the reversal starts from one or both ends. Finally, for a low-resolution model in the form of a single spin with an anisotropic potential, the bimodal distribution is an artifact of the definition of a switching event: the result of the spin precessing close to \(M_z = 0\). While the zero- and one-dimensional models display bimodal switching-time distributions, the mechanisms are different for the three-dimensional model. Only the latter captures the mechanism that is most interesting from an experimental and device-application point of view.

\(^1\)Supported by NSF grant DMR-0444051.

Monday, March 10, 2008 8:00AM - 10:48AM — Session A16 DBP DPOLY: Dynamics of Nucleic Acids Morial Convention Center 208

8:00AM A16.00001 Biochemistry on a leash: A mechanism for ligand recruitment via tethered binding sites, DANIEL REEVES, KEITH CHEVERALLS, JANNE KONDEV, Brandeis University — The diffusion limited reaction rate for ligand-receptor systems is typically estimated as the rate at which the ligand stumbles upon the receptor site by three-dimensional Brownian motion. We consider a mechanism that improves upon this limiting rate by placing a binding site on a flexible polymer. The tethered binding site explores the vicinity of the receptor site via polymer diffusion. After binding the ligand, the tether directly transfers it to the receptor site. This is in contrast with existing models, which involve non-specific binding that confines the ligand to lower-dimensional diffusion. The proposed mechanism may be relevant to the biological actin capping protein formin, which increases actin polymerization rates when bound to the growing tip of actin filaments.

8:12AM A16.00002 Backtracking and error correction in DNA transcription, MARGARITIS VOLIOTIS, School of Computing and Department of Applied Mathematics, University of Leeds, NETTA COHEN, School of Computing, University of Leeds, CARMEN MOLINA-PARIS, Department of Applied Mathematics, University of Leeds, TANNIEMOLA LIVERPOOL, Department of Mathematics, University of Bristol — Genetic information is encoded in the nucleotide sequence of the DNA. This sequence contains the instruction code of the cell—determining protein structure and function, and hence cell function and fate. The viability and endurance of organisms crucially depend on the fidelity with which genetic information is transcribed/translated (during mRNA and protein production) and replicated (during DNA replication). However, thermodynamics introduces significant fluctuations which would incur massive error rates if efficient proofreading mechanisms were not in place. Here, we examine a putative mechanism for error correction during DNA transcription, which relies on backtracking of the RNA polymerase (RNAP). We develop an error correction model that incorporates RNAP translocation, backtracking pauses and mRNA cleavage. We calculate the error rate as a function of the relevant rates (translocation, cleavage, backtracking and polymerization) and show that the its theoretical limit is equivalent to that accomplished by a multiple-step kinetic proofreading mechanism.

8:24AM A16.00003 Effects of crosslinks on motor-mediated filament organization\(^1\), IGOR ARANSON, FALKO ZIEBERT, Argonne National Laboratory, LEV TSIMRING, University of California, San Diego — Crosslinks and molecular motors play an important role in the organization of cytoskeletal filament networks. Here we incorporate the effect of crosslinks into our model of polar motor-filament organization, through suppressing the relative sliding of filaments in the course of motor-mediated alignment. We show that this modification leads to a nontrivial macroscopic behavior, namely the oriented state exhibits a transverse instability in contrast to the isotropic instability that occurs without crosslinks. This transverse instability leads to the formation of dense extended bundles of oriented filaments, similar to recently observed structures in actomyosin. This model also can be applied to situations with two oppositely directed motor species or motors with different processing speeds.

\(^1\)This work was supported by the US DOE, grant DE-AC02-06CH11357.

8:36AM A16.00004 Collective alignment of polar filaments by molecular motors\(^1\), IGOR ARANSON, Argonne National Laboratory — We study the alignment of polar biofilaments, such as microtubules and actin, subject to the action of multiple molecular motors attached simultaneously to more than one filament. Focusing on a paradigm micromechanical model of only two filaments interacting with multiple motors, we were able to investigate in detail the dynamics of the filaments’ alignment. While almost no alignment occurs in the case of a single motor, we show that the filaments become perfectly aligned due to the collective action of the motors working together. Our studies revealed that the the alignment time is governed by the magnitude of the fluctuations in the motor force.

\(^1\)This work was supported by the US DOE, grant DE-AC02-06CH11357.

8:48AM A16.00005 Detecting cooperative sequences in the binding of RNA Polymerase-II, KIMBERLY GLASS, University of Maryland, JULIAN ROZENBERG, National Cancer Institute (NIH), MICHELLE GIRVAN, WOLFGANG LOSERT, ED OTT, University of Maryland, CHARLES VINSON, National Cancer Institute (NIH), UMD/NIH SYSTEMS BIOLOGY COLLABORATION COLLABORATION — Regulation of the expression level of genes is a key biological process controlled largely by the 1000 base pair (bp) sequence preceding each gene (the promoter region). Within that region transcription factor binding sites (TFBS), 5-10 bp long sequences, act individually or cooperate together in the recruitment of, and therefore subsequent gene transcription by, RNA Polymerase-II (RNAP). We have measured the binding of RNAP to promoters on a genome-wide basis using Chromatin Immunoprecipitation (ChiP-on-Chip) microarray assays. Using all 8-base pair long sequences as a test set, we have identified the DNA sequences that are enriched in promoters with high RNAP binding values. We are able to demonstrate that virtually all sequences enriched in such promoters contain a CpG dinucleotide, indicating that TFBS that contain the CpG dinucleotide are involved in RNAP binding to promoters. Further analysis shows that the presence of pairs of CpG containing sequences cooperate to enhance the binding of RNAP to the promoter.
9:00AM A16.00006 Dynamic self-assembly of nanocomposite ring structures through the interaction of thermodynamic and energy-dissipating processes. HAIQING LIU, ERIK SPOERKE, MARLENE BACHAND, STEVEN KOCH, BRUCE BUNKER, GEORGE BACHAND; Sandia National Laboratories — Self-assembly of nanostructured materials occurs in thermodynamic and energy-dissipating systems. We've described a unique self-assembly scheme in which non-equilibrium nanocomposites are formed by the interaction of energy dissipation and thermodynamics. Three distinct composite structures (mobile linear, rotating circular and immobile aggregated composites) are formed when streptavidin-coated quantum dots are introduced to biotinylated microtubules that are being transported by kinesin. The circular nanocomposites occur only in a delicately balanced regime when thermodynamic and energy-dissipating components interact cooperatively. Linear translation and axial rotation of microtubules drive the formation of non-equilibrium structures which ultimately define the structural shape and rotational direction. Disassembly of these composites occurs spontaneously, as well as induced by the addition of free biotin. Exploitation of dynamic self-assembly promises nanostructured materials with revolutionary behaviors that are unattainable through conventional self-assembly.

*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, or the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:12AM A16.00007 How Large are Cooperative Effects in Hydrogen Bonded Molecular Chains? MARTIN FUCHS, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany, JOEL IRETA, Univ. Autonoma Metropolitana Iztapalapa, Mexico — Intermolecular hydrogen bonds play an eminent role in a wide range of materials. In particular, they are critical for the secondary structure stabilization of biopolymers like proteins and nucleic acids. Arrays of hydrogen bonds (hbs), such as in chains or helices, often display a cooperative strengthening of the individual hbs. This cooperativity is crucial for understanding the stability and properties of hydrogen bonded materials. Here we investigate the hb cooperativity in model chains of HCl, HF, HCN, formamide, and 4-pyridone, i.e. molecules forming weak to strong hbs. We calculate the hb strength of infinitely long chains using density-functional theory (DFT) with the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA). We show that for large intermolecular separations, the hbs in the infinite chain strengthen by 20% over the respective molecular dimers, consistent with dipolar electrostatics [1]. At the equilibrium separation, the hbs strengthen significantly further (up to 260% for HF), with additional stabilization from induced dipolar interactions. Comparing with results from higher-level calculations (MP2 and quantum Monte Carlo) we find that DFT faithfully describes the cooperativity in these systems in which the hbs are close to linear. [1] P.B. Allen, J. Chem. Phys. 120, 2951 (2004)

9:24AM A16.00008 Single stranded DNA hairpin loop kinetics: A Brownian dynamics study. MARTIN KENWARD, KEVIN DORFMAN, University of Minnesota — The dynamics of single stranded DNA (ssDNA) molecules play a role in a number of biological functions and have a found uses in several microfluidic applications. In particular, ssDNA having complementary sequences at their ends can form hairpin loops in which the complementary sections bind to one another. The appearance of these loops and fluctuations between open and closed states depend on a number of variables including: the degree of complementarity of the end sequences, the species, temperature and strength of hydrogen bonding and base stacking.

In this study, we present a Brownian dynamics model which is used to examine the kinetics of the hairpin loop formation. We present results for the melting behavior of hairpins as a function of temperature and other system parameters. We also present results for the kinetic rate constants $k_-$ and $k_+$ corresponding to the open-closed and closed-open transitions respectively.

9:36AM A16.00009 Statistical Analysis of the Chemotactic Motility Cycle of Amoeboid Cells. BALDOMERO ALONSO-LATORRE, JUAN C. DEL ALAMO1, RUEDI MEILI, RICHARD A. FIRTEL, JUAN C. LASHERAS, University of California, San Diego — Amoeboid motility results from the repetition of stereotypic steps that produce quasi-periodic oscillations of cell length and speed. We characterize the steps of the motility cycle of Dictyostelium cells crawling on elastic substrates by analyzing their traction forces. Using a high-resolution force cytomtery method for wild type and mutant cells, we find that the time evolution of the traction forces is quasi-periodic, with a period $T$ that correlates strongly with the cell speed $V$ according to a simple law $VT=L$. The constant $L$ is the distance traveled per cycle. The magnitude of the traction forces exerted by the cells does not correlate with the cell speed, suggesting that the speed of migration is determined by the ability of the cell to rapidly repeat the phases of the motility cycle. Phase average statistics allow us to combine time sequences of force maps derived from different cells to obtain a spatio-temporal representation of a canonical motility cycle divided into four steps: protrusion, contraction, retraction and relaxation. We find that myosin II-dependent contraction is present in all steps of the wild-type cycle, including protrusion.

1Partially supported by Spanish MEC (Fulbright Program)

9:48AM A16.00010 Force generated by polymerization of actin filaments. CORALINE BRANGBOURG, OLIVIA DU ROURE, EMMANUELLE HELFER, MÁRC FERMIGIER, MARIE-FRANCE CARLIER, JÉRÔME BIBETTE, JEAN BAUDRY, Laboratoire des Molécules et d’assemblage Protéique, Université Paris-Sud, CNRS, Gif-sur-Yvette, France — Actin polymerization drives protrusions at the cell surface and leads to cell motility. Using magnetic colloids, we measure how the chemical reaction of polymerization generates mechanical forces. We detail in particular the force-velocity relation of growing actin filaments; and how the scaling force is affected by the mean number of filaments between two beads.

10:00AM A16.00011 Probing Brownian Motion of an Ellipsoid with an External Force. SHAO-QING ZHANG, WU-PEI SU, Dept. of Physics, Univ. of Houston, TX 77204 — Brownian motion has translational and rotational degrees of freedom. Anisotropy in the shape of a Brownian particle leads to dissipative coupling between translational and rotational motion. However, the coupling effects, which depend on the initial orientation of an ellipsoid, cannot be detected by most typical experimental techniques. To surmount the hurdle between theoretical predictions and experimental measurements, we present a theoretical scheme for uncovering the translation-rotation coupling by applying a constant external force to an ellipsoid in a two-dimensional suspension. The geometry of the ellipsoid can be determined using only the first two cumulants. An anisotropy-isotropy alternation is found in the cumulant series. We also discuss the probability distribution function (PDF) of lab-frame displacements to gain insight into the significance of anisotropy of a Brownian particle in diverse environments.

10:12AM A16.00012 Probing Protein Conformations at the Oil-water Interface Using Single-Molecule Force Spectroscopy. AHMED TOUHAMI, MARCELA ALEXANDER, MILENA CORREDIG, JOHN DUTCHER, University of Guelph — The present work aims at a deeper understanding of the conformational changes in Beta-lactoglobulin (BLG) protein adsorbed onto the oil-in-water emulsion interfaces due to variations in pH. Mechanical unfolding of BLG by AFM-single-molecule force spectroscopy (AFM-SMFS) was performed on single oil droplets that were mechanically trapped in a polycarbonate filter. The changes in the contour length upon each unfolding event were determined by fitting the WLC model of polymer elasticity to each of the BLG peaks. Our results show clearly that at pH 2.5 BLG exists as a dimer in which each monomer is similar to two Immunoglobulin domains. At pH 6.8 BLG on the oil droplets adopts a conformation consisting of domains with a contour length of 11 nm. Furthermore, at pH 9 the interactions between the AFM tip and the BLG layer on the oil droplet surface are dominated by a huge repulsion due to the highly negatively charged BLG layer. This study demonstrates a novel application of AFM-SMFS to investigate the underlying mechanisms by which proteins can be used to stabilize food products.

Comparing with results from higher-level calculations (MP2 and quantum Monte Carlo) we find that DFT faithfully describes the cooperativity in these systems in which the hbs are close to linear. [1] P.B. Allen, J. Chem. Phys. 120, 2951 (2004)
10:24AM A16.00013 Structural motifs of biomolecules¹, HOANG TRINH, JAYANTH BANVAR, Penn State University, University Park, PA 16801, USA, AMOS MARITAN, CHIARA POLETTA, ANTONIO TROVATO, Università di Padova, 35131 Padova, Italy, JOHN MADDOCKS, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland, ANDREJ STASIAK, University of Lausanne, CH-1015 Lausanne, Switzerland — Biomolecular structures are assemblies of emergent anisotropic building modules such as uniaxial helices or biaxial strands. We provide an approach to understanding a compact phase of matter that is occupied by proteins and DNA. This phase, which is in some respects analogous to the liquid crystal phase for chain molecules, stabilizes a range of shapes that can be obtained by sequence-independent interactions occurring intra- and intermolecularly between polymeric molecules. We present a singularity free self-interaction for a tube in the continuum limit and show that this results in the tube being positioned in the marginally compact phase. Our work provides a unified framework for understanding the building blocks of biomolecules.


10:36AM A16.00014 Instabilities of ordered chiral active suspensions, TAPAN ADHYAPAK, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012 INDIA, DAVIDE MARENUZZO, The School of Physics, The University of Edinburgh, James Clerk Maxwell Building, The Kings Buildings, Mayfield Road, Edinburgh EH9 3JZ, UK, SRIRAM RAMASWAMY, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012 INDIA — Suspensions of actively contractile or tensile filaments with simple orientational order are hydrodynamically unstable. Here we study, analytically as well as numerically, the manner in which the presence of cholesteric order competes with this instability.

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8:00AM A17.00001 The Significance of Replication, MICHAEL C.H. MCKRUBLE, FRANCIS L. TANZELLA, SRI International, Menlo Park, CA 94025, VITTORIO VIOLANTE, ENEA, Frascati, Italy — Much has been made of an apparent lack of reproducibility in so called “cold fusion” experiments. In this paper we will demonstrate that this failure, while real, was the result of inability to meet critical threshold criteria: a thermodynamic loading, dynamic flux and disequilibrium trigger. Recent experiments, performed independently at SRI and ENEA, have successfully replicated powerful excess heat results obtained initially by Enertics in Israel. This success and high levels of experiment reproducibility are attributed to two critical factors that allow these threshold barriers to be surpassed: i) achievement and maintenance of a high level of control of the metallurgy of the bulk palladium metal host and the cathode surface morphology, guided by initial studies at ENEA and the University of Rome, ii) use of a novel non steady-state cathode current stimulus, proposed and developed by Enertics. With simultaneous high deuterium loading and high flux, excess heat effects were measured in both isoperibolic and Mass Flow calorimeters at factors several times greater than the electrical input power and several orders of magnitude larger than the sum of all conceivable chemical reactions.

8:12AM A17.00002 Public-Interest and Level-of-Evidence Considerations in Cold Fusion Public Policy, THOMAS GRINSHAW, LBJ School of Public Affairs, The University of Texas at Austin — Cold fusion (CF) protagonists and antagonists would no doubt agree that scientific processes have been challenged in the CF case. The public interest in CF turns on two questions: What are the potential benefits? What is the probability that CF is “real”? Potential benefits have been agreed on since CF announcement in 1989. The probability of CF reality may be assessed based on level of evidence (LoE): preponderance of evidence (PoE); clear and convincing evidence (CCE); and beyond a reasonable doubt (BRD). PoE, from civil law, indicates a probability of 50% or higher. BRD, from criminal law, has a probability approaching 90%. CCE, in between, thus has a 70-75% probability. CF experimental evidence, based on: 1) initial affirmations, 2) the large number of corroborations since marginalization, and 3) particularly (BRD). PoE, from civil law, indicates a probability of 50% or higher. BRD, from criminal law, has a probability approaching 90%. CCE, in between, thus has a 70-75% probability. CF experimental evidence, based on: 1) initial affirmations, 2) the large number of corroborations since marginalization, and 3) particularly 70-75% probability. CF experimental evidence, based on: 1) initial affirmations, 2) the large number of corroborations since marginalization, and 3) particularly demonstrative experiments, reasonably indicates at least a PoE level of evidence for excess heat. A case can also be made for a CCE (but probably not for a BRD) LoE. In either the PoE or CCE scenario a clear need is demonstrated for change in policy toward CR, given its potential benefits to humanity.

8:24AM A17.00003 Anomalous Radiation Produced by Glow Discharge in Deuterium Containing Oxygen, EDMUNDO STORMS, BRIAN SCANLAN, KivaLabs, LLC, 2140 Paseo Ponderosa, Santa Fe NM 87501 — Electromagnetic Radiation (EMR) and anomalous radiation (potentially produced by nuclear reactions, involving high energy particles), in a low-voltage discharge in a gas containing deuterium was measured using a Geiger counter located within the apparatus. This radiation is found to consist of energetic particles that are produced only when the voltage is above a critical value. In addition, the emission is very sensitive to the presence of oxygen in the gas. The intensity of the reaction producing the radiation could be fit by a power function when compared to the applied voltage. The effect of EMR and other sources of noise that might be attributed to the anomalous radiation are discussed.

8:36AM A17.00004 Low Energy Nuclear Reaction Products at Surfaces, DAVID J. NAGEL, The George Washington University — This paper examines the evidence for LENR occurring on or very near to the surface of materials. Several types of experimental indications for LENR surface reactions have been reported and will be reviewed. LENR result in two types of products, energy and the appearance of new elements. The level of instantaneous power production can be written as the product of four factors: (1) the total area of the surface on which the reactions can occur, (2) the fraction of the area that is active at any time, (3) the reaction rate, that is, the number of reactions per unit active area per second, and (4) the energy produced per reaction. Each of these factors, and their limits, are reviewed. A graphical means of relating these four factors over their wide variations has been devised. The instantaneous generation of atoms of new elements can also be written as the product of the first three factors and the new elemental mass produced per reaction. Again, a graphical means of presenting the factors and their results over many orders of magnitude has been developed.

8:48AM A17.00005 Evidence and Theory for Cluster Reactions in LENRs, GEORGE H. MILEY, HEINZ HORA¹, ANDREI LIPSON, PRAJAKTI JOSHI SHRESTHA, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois — A distinctive array reaction products attributed to nuclear reactions was observed earlier in the "Patterson" flowing packed-bed type electrolytic cell experiments using multilayer thin films of metals on mm-size plastic beads. The swimming electron layer and a new magic number theory were proposed to explain this. More recently these theories have been expanded into a “D-Pd-D cluster” model to explain a wider range of transmutation experiments. This cluster model is consistent with certain measurements of energetic charged-particle emission during thin film electrolysis, with observations suggesting localized reactions and also with x-ray production during plasma bombardment experiments. The cluster reaction concept and supporting experimental data will be discussed in this presentation. In addition to explaining , if understood and optimized, cluster reactions could lead to an important new power source based on Low Energy Nuclear Reactions (LENRs). A conceptual power cell based on a novel electrode design that promotes cluster reactions is presented.

¹Dept. Theoretical Physics, University of NSW, Sydney 2052, Australia
9:00AM A17.00006 Compound Nucleus Reactions in LENR, Analogy to Uranium Fission , HEINRICH HORA, GEORGE MILEY1, KARL PHILBERTH2. Department of Theoretical Physics, University of New South Wales, Sydney 2052, Australia — The discovery of nuclear fission by Hahn and Strassmann was based on a very rare microanalytical result that could not initially indicate the very complicated details of this most important process. A similarity is discussed for the low energy nuclear reactions (LENRs) with analogies to the yield structure found in measurements of uranium fission. The LENR product distribution measured earlier in a reproducible way in experiments with thin film electrodes and a high density deuteron concentration in palladium has several striking similarities with the uranium fission fragment yield curve. This comparison is specifically focussed to the Maruhn-Greiner local maximum of the distribution within the large-scale minimum when the fission nuclei are excited. Implications for uranium fission are discussed in comparison with LENR relative to the identification of fission a hypothetical compound nuclear reaction via a element $^{306}_{126}$ with double magic numbers.

1University of Illinois, Urbana, IL, USA  
2Thanning, 82544 Egling, Germany

9:12AM A17.00007 New Mechanism for Explaining LENR and Certain forms of Technological and Natural Catastrophes , FANGIL GAREEV, Joint Institute for Nuclear Research, Dubna, Russia — We propose a new mechanism for low energy nuclear reactions (LENR): cooperative resonance processes involving the whole the system - nuclei + atoms + condensed matter can occur at a smaller threshold energies than the corresponding ones on free constitutuents. The cooperative processes can be induced and enhanced by low energy external fields. The excess heat is the emission of internal energy and transmutations at LENR are the result of a redistribution of internal energy of the whole system. The lack of financial support and ignorance by mainstream physicists has resulted in the LENR field not being accepted. We postulate that LENR can lead to catastrophes, potentially including, the runaway event involving the reactor at the Chernobyl Nuclear Power Plant, the explosion of the twin towers during the 11 September 2001 World Trade Center collapse, in New York, the explosion of transformers in Moscow, catastrophes of submarines, and other phenomena associated with a cooperative resonance synchronization mechanism.

9:24AM A17.00008 Predictability of Theory, and Collaboration with Experimentalists in CMNS, XING ZHONG LI, Department of Physics, Tsinghua University, Beijing 100084, China — Condensed Matter Nuclear Science has confirmed 2 outstanding experimental results: 144.5W of continuous “Excess Heat” in 10 minutes(ICCF-3,1992) and the nuclear transmutation induced by deuterium flux on the Pd surface (ICCF-8, 2000). Theory predicted neutron emission based on the previous beam-target experiments. It was a wrong guidance, because there was no “commensurate neutron” detected. The collaboration with experimentalists helped theorist to modify their prediction in the past 19 years. Theorists might imagine that “high loading ratio” was necessary; then, the experiments said “deuterium flux was more important.” Resonant tunneling theory imagined again “any resonance in inelastic scattering (nuclear reaction) had to be accompanied by a resonance in elastic scattering (diffusion); hence, a peak in excess heat should be correlated with a peak in deuterium flux.” The experiments seem to confirm this imagination. The next 2 predictions are: (1) Adjusting the loading rate to form a steady state for resonant tunneling;(2)Neutroin detection from this steady state to confirm its nuclear nature.

9:36AM A17.00009 Comparison of SPAWAR Co-deposition Experimental Data and Competing Condensed Matter Nuclear Science Theories, LAWRENCE P.G. FORSLEY, JWK Technologies Corporation, 7617 Little River Turnpike Suite 1050, Annandale, VA 22003, PAMELA MOSIER-BOSS, Space Warfare Systems Center, San Diego — The SPAWAR PdD co-deposition protocol has been replicated in several laboratories and shown to produce apparent nuclear tracks in solid-state CR-39 detectors. Additional spectroscoptic gamma ray measurements have been carried out using either high resolution, cryogenically cooled germanium or lower resolution sodium iodide detectors. These results are at odds with many of the competing theories in this field, suggesting the need to acquire additional temporally and spectrally resolved nuclear data.

9:48AM A17.00010 Multiple Etching of CR-39 Nuclear Track Detectors used in SPAWAR Co-Dep Experiment, PAMELA MOSIER-BOSS, Space Warfare Systems Center, San Diego, LAWRENCE P.G. FORSLEY, JWK Technologies Corporation, 7617 Little River Turnpike Suite 1050, Annandale, VA 22003 — Previously published results involving the use of the solid state track detectors, CR-39, have brought into question whether or not purported tracks are of nuclear origin. One method of determining this is to serially etch and scan these track detectors so as to determine the approximate depth of the tracks. This method, coupled with a computer code incorporating bulk and track etching rates in CR-39 for alpha particles, gives good agreement with tracks seen in SPAWAR co-deposition experiments as compared to known alpha sources.

10:00AM A17.00011 Spatial and Temporal Resolution of Three Sites Characterizing Lattice-Assisted Nuclear Reactions (LANR) , MITCHELL SWARTZ. JET Energy, Inc. Wellesley, MA 02481 — We present developing evidence that three different sites (physical locations in the solid state) are involved in lattice-assisted nuclear reactions (LANR). By expanding the equation first developed by Prof. David Nagel at ICCF-13, we correlate observations of excess heat and de novo helium-4 production to three different physical locations and to the optimal operating points (OOPs) which are now known to characterize LANR system. This observation will be shown to be consistent with our previous reports of distinct time constants which characterize the tardive thermal power regime (“heat after death”), which results after all input electrical power is terminated to an active LANR device.

1Nagel, D., “Rates for LENRs at Surfaces”, ICCF-13  
interstitial Ds. Large "cage" of CD's forms with a definite phase and zero entropy, trapping a "gas" of non-coherent Ds. In our D-Pd-D cluster theory this explains D-Pd-D cluster reactions in certain cold fusion experiments.

This compares with best plasma fusion runs of 16 MW of fusion heat for \( \leq 1s \) (\( \leq 1.6 \times 10^7 \) J). The fusion heat was less than the input energy. In 2004, Arata and Zhang pressure-loaded \( \text{ZrO}_2 + \text{nanoPd} \) with \( D_2 \) at \( 140 \, ^\circ\text{C} \) and produced an estimated steady 0.6 W of fusion heat. The ionic oxide + nanometal composites absorb abnormal amounts of hydrogen gas.

An ensemble of D atoms loaded into Pd can assume two different configurations coupled with the intrinsic EM field. A coherent state forms above critical density and temperature thresholds. This new state has lower energy than the Pd lattice. In 2004, Arata and Zhang pressure-loaded \( \text{ZrO}_2 + \text{nanoPd} \) with \( D_2 \) at \( 140 \, ^\circ\text{C} \) and produced an estimated steady 0.6 W of fusion heat. The ionic oxide + nanometal composites absorb abnormal amounts of hydrogen gas.

Cold Fusion Reactions, LINCHON WU, GEORGE MILEY, University of Illinois, NPRE Department, 103 S. Goodwin Ave — G. Preparata earlier proposed a radical new QED theory, and had just begun application to cold fusion prior to his untimely death. Cold Fusion Reactions, LINCHON WU, GEORGE MILEY, University of Illinois, NPRE Department, 103 S. Goodwin Ave — G. Preparata earlier proposed a radical new QED theory, and had just begun application to cold fusion prior to his untimely death.

8:36AM A18.00002 Microrheology of Nanospheres in Rod Suspensions, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Many biological processes and applications involve the motion of small (nanoscale) spherical particles through a dense (typically) semiflexible polymer matrix. While much theoretical work has characterized the motion of such particles in the limit of its size being much larger than the mesh size of the matrix, very limited understanding exists of the (more biologically relevant) crossover regime to the case where the particle size becomes comparable to the mesh size. Recently we have developed a new computer simulation method to simulate the dynamical and rheological properties of colloid suspensions of a variety of complex fluids. We first present the results of its generalization to the dynamics and linear rheological properties of dilute, semiflexible and concentrated rods suspensions in a simple fluid. Subsequently, we use this method to characterize the mobility and diffusive dynamics of nanoscale spheres in rod matrices, while paying special attention to the length scales of the fluid which characterize the hydrodynamic screening and overall viscous motion.

8:48AM A18.00003 Peptide binding to sheet silicate and metal nanoparticles: Insight from atomistic simulation, RICHARD A. VAIA, RAJESH R. NAJK, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Short peptides (8 to 12 amino acids, excluding Cys) bind selectively to nanoscale particles composed of Au, Pd, and montmorillonite depending on the sequence of amino acids, as evidenced by laboratory screening of several billion peptides. The molecular reasons for binding versus non-binding and the specificity toward a certain surface are analyzed by molecular dynamics (MD) simulations. RICHARD A. VAIA, RAJESH R. NAJK, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Using a coarse grained description, we study stability of the structure and dynamics of several peptide chains (A3, Fig, Pro10, Gly10, Pd2, Pd4) at gold surfaces on a cubic lattice. Although the structural details within the amino acid groups are ignored, the specificity of their interactions is incorporated in our computer simulation modeling of these peptide chains on a cubic lattice. Appropriate coarse-grained interactions (Lennard-Jones) among the amino acid nodes, solvent, and the gold surface with different strength are guided by the atomistic simulations and X-ray crystallographic data; the molecular weight of each amino acid groups is also considered. Peptide chains execute their stochastic motion and their proximity to the generic gold surface is monitored. Mobility of each amino acid (node), its energy, and correlations to their neighboring constituents are analyzed. Some of these results are consistent with the atomistic simulation.

9:00AM A18.00004 Adsorption-desorption of peptide chains on Au surface by a coarse-grained Monte Carlo simulation, RAS B. PANDEY, University of Southern Mississippi, HENDRIK HEINZ, University of Akron, LAWRENCE R. DRUMM, RICHARD A. VAIA, RAJESH R. NAJK, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Using a coarse grained description, we study stability of the structure and dynamics of several peptide chains (A3, Fig, Pro10, Gly10, Pd2, Pd4) at gold surfaces on a cubic lattice. Although the structural details within the amino acid groups are ignored, the specificity of their interactions is incorporated in our computer simulation modeling of these peptide chains on a cubic lattice. Appropriate coarse-grained interactions (Lennard-Jones) among the amino acid nodes, solvent, and the gold surface with different strength are guided by the atomistic simulations and X-ray crystallographic data; the molecular weight of each amino acid groups is also considered. Peptide chains execute their stochastic motion and their proximity to the generic gold surface is monitored. Mobility of each amino acid (node), its energy, and correlations to their neighboring constituents are analyzed. Some of these results are consistent with the atomistic simulation.

9:12AM A18.00005 Characterization of the translocation of polymers driven through nanopores using molecular dynamics simulations, HENDRICK DE HAAN, GARY W. SLATER, University of Ottawa — The passage of a polymer through a narrow pore (translocation) is a fundamental process with a wide range of biological applications. In particular, threading DNA through nanopores promises to have important implications for the next generation of DNA sequencing techniques. In this work, simulations of the translocation of polymers being driven through a narrow, short nanopore are conducted via the Espresso Molecular Dynamics simulation package using the Lattice-Boltzmann algorithm to include hydrodynamics. In this talk, results from simulations in which an external field is applied within the pore or to one end of the polymer are presented and compared. Characterization of the scaling of the translocation time with the number of monomers as well as details of the anomalous diffusion exhibited by the translocation coordinate will be given.

9:24AM A18.00006 Coupling of atomistic and mesoscopic scales: visualizing the translocation of biopolymers through nanopores, MARIA FYTA, Department of Physics, Harvard University, SIMONE MELCHIONNA, INF-M-SOFT, Department of Physics, Universita di Roma La Sapienza, P.le A. Moro 2, 00185 Rome, Italy, MASSIMO BERNASCHI, Istituto Applicazioni Calcolo, CNR, Viale del Policlinico 137, 00161, Roma, Italy, ETHEMIMOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA, SAURO SUCCI, Istituto Applicazioni Calcolo, CNR, Viale del Policlinico 137, 00161, Roma, Italy — We investigate the process of biopolymer translocation through a narrow pore using a multiscale approach, which combines Langevin Molecular-Dynamics with a mesoscopic Lattice-Boltzmann method for the solvent dynamics. We analyze the statistical features of the translocation process through extensive simulations over various polymer conformations and strengths. The translocation time obeys a power law dependence to the polymer length with an exponential factor of the order of 1.28 ± 0.01 for very good agreement with experiments of DNA translocation through solid state pores. We focus on the morphological aspects of the translocation dynamics, the folding behavior of the translocating molecule and the associated cooperation of the surrounding solvent, and report the first computational evidence of quantized current blockades.

9:36AM A18.00007 Coarse-Grained Kinetic Modeling of Polymer Networks with Non-Affine Slip-Tube Behavior and Heterogeneous Microstructure, BRIAN PASQUINI, FERNANDO ESCOBEDO, YONG LAK JOO, Department of Chemical and Biomolecular Engineering, Cornell University — Elements of existing entanglement network models have been extended to better account for non-affine slip-tube behavior and to incorporate the effect of heterogeneous spatial domains. Starting with the Density Cloud Model (DCM) framework from Terzis et al., an entanglement bond potential acting at each entanglement point is introduced. This potential mimics the non-affine tethering from network theories, and in combination with slippage accurately reproduces Non-Affine Slip-Tube behavior. This framework can easily be extended to study the effect of polymer architecture on the mechanical response of the resulting networks. Secondly, the temporary bond from the model of Terzina and Smith is combined with the DCM framework to simulate rigid domains within a matrix of soft polymer network. The modulus of the additional bonds sets the elastic properties of the rigid domain, while DCM entanglement relaxation assures that local deformation remains consistent with the bulk polymer density. The effect of rigid domain size on initial modulus is reported.

9:48AM A18.00008 Simulating thermal transport in high contrast composite media, HARSHADEWA S. GUWADARANA, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, DIMITRIOVS P. PAPAVASSILIOU, Department of Chemical Engineering, University of Oklahoma — In dealing with transport in composites systems, high contrast materials pose a special problem for numerical simulation: the time scale or step size in the high thermal conductivity material must be much smaller than the low conductivity material. High conductivity inclusions can be treated as having an infinite conductivity, removing the need to model transport within the high conductivity inclusions. We develop a random walk algorithm to model thermal transport in composites with high conductivity. We observed the standard random walk algorithm leads to non uniform temperature distribution at the vicinity of the high conductivity inclusion violating the second law of thermodynamics. We show how a standard random walk algorithm can be altered to improve speed while still preserving the second law of thermodynamics. We demonstrate the algorithm in 1D and 3D systems.
10:00AM A18.00009 Predictive Morphology Models for Crystalline Polymers1,2 — JACOB HARVEY, ZHICHENG XIAO, YVONNE AKPALU, Department of Chemistry & Chemical Biology, Rensselaer Polytechnic Institute — Modeling of small-angle scattering data provides information on heterogeneities on sizes on the order of 10 Angstroms and larger. The typical size, shape and arrangement of the heterogeneity can be determined by applying models to the scattering intensity I(q). When there is a distribution in the size of structures present and when a system is densely packed, it is likely that models that can be used for analysis may not provide a unique description of the structure. With the recent interest developing in predicting models for molecular level control over the properties of polymers, it is desirable to determine all unique structural and morphological contributions to a scattering curve without assuming a model. However, by using a multi-scale approach (i.e. light and X-ray scattering spanning multiple size scales), it may be possible to build unique models for crystalline polymers. We will show that hybrids of statistical methods can be used to decouple scattering data into unique structural components. We will show how our approach can be used to discover analytical models and to develop a set of descriptors that can be used to predict scattering curves for several other polymers that share a similar structure or crystallization condition.

1 Thanks to NSF and DOE for financial support.

10:12AM A18.00010 Coarse-grained Molecular Dynamics Simulations and Analysis of Poly(L-lactic Acid) (PLLA) Melt — Gaurav Manik, HemanT Nanavati, Chemical Engg. Department, Indian Institute of Technology Bombay, Mumbai-400076, India, Upendra Natarajan, Chemical Engg. Department, Indian Institute of Technology Madras, Chennai-600036, India — We present coarse-grained (CG) MD simulations of the melt structure of PLLA, a very useful biodegradable polymer. Our CGMD simulations consider entire repeat unit as a one bead and use IBI scheme. The CG potentials and forces are obtained after performing atomistic MD of 52 PLLA tetramer molecules and employing the probability distributions for the corresponding CG lengths, angles, dihedrals, and the radial distribution function. The initial energy-minimized samples are equilibrated for density in NPT ensemble, followed by structural equilibration. The simulated characteristic ratio (2.13) and density (1.123g/cc) at 450K are in excellent agreement with the expt. values1 of 2.2 and 1.152g/cc at 413K. The equilibrated structures were analyzed for primitive path properties, tube diameter, , entanglement length, , etc., using Kroger’s Z-code2. This yields for longest chains (N=1000) and compare favorably with expt. values.1, 55 and 47.7Å (413K).


10:24AM A18.00011 Modeling the Thermodynamics of the Interaction of Nanoparticles with Cell Membranes1 — Valerie Ginzburg, Sudhakar BalljaPalli, The Dow Chemical Company — Interactions between nanoparticles and cell membranes may play a crucial role in determining the cytotoxicity of nanoparticles as well as their potential application as drug delivery vehicles or therapeutic agents. It has been shown that such interactions are often determined not by biochemical but by physico-chemical factors (e.g., nanoparticle size, hydrophobicity, and surface charge density). Here, we propose a mesoscale thermodynamic model describing the transitions in membrane morphology observed after exposure to various types of nanoparticles. Our simulations demonstrate under which conditions (determined by particle size and hydrophilic/hydrophobic interactions) the particles can adsorb into the membrane or compromise the membrane integrity to result in the formation of nano-sized holes. The model could be refined to include a more accurate description of various phospholipid membranes, and its results could be applied in the design of specific nanoparticles for various biomedical applications.

1 This work is supported by The Dow Chemical Company

10:36AM A18.00012 Structure and dynamics of a model polymer nanocomposites — Monojoy Goswami, Bobby Sumpter, Oak Ridge National Laboratory — We investigate the structure and the dynamics of a model polymer nanocomposite (PNC) through molecular dynamics (MD) simulations in the canonical ensemble (NVT). Several computer experiments have been carried out at different temperatures for different Lennard-Jones well-depth and filler volume fraction. We studied the real space pair correlation functions and collective scattering structure factors of the PNC melt. This structural analysis has been compared with the previous theoretical and experimental works. The reinforcement of the nanocomposite have been investigated using stress-stress autocorrelation (σxy(t)) function for different temperatures. At lower temperatures, σxy(t) shows strong reinforcement of the nanocomposite while at higher temperatures it relaxes quite fast. Diffusion of nanoparticles in the composite has been investigated and compared with earlier works. The effect of sizes and shapes of the nanoparticles has also been investigated in this work.

10:48AM A18.00013 Strategies for design of polymeric nanoparticle — JiWu Liu, Michael Mackay, Phillip Duxbury, Michigan State University — Recently polymer nanoparticles have been synthesized using single chains as macromolecular precursors, providing unprecedented control of nanoparticle size and function. We present the results of molecular dynamics simulations which provide detailed insight into the formation kinetics of specific polymeric nanoparticles and which also predict design strategies for formation of interesting new targets. Nanoparticles are formed through chemical crosslinking which is possible when reactive species on the chain backbone are in close proximity. Since the chemical crosslinking is highly irreversible, nanoparticles formed in this way do not unfold on heating, in contrast to the familiar case of thermal denaturing of proteins. Synthesis of precursors with an alphabet of orthogonal crosslinkers provides a rich phase space for design of polymeric nanoparticles. For example, our simulations indicate that an alphabet of three orthogonal crosslinkers enables self-assembly of two-faced or Janus nanoparticles and a variety of other morphologies.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A19 DCMP: Magnetic and Superconducting Properties — Morial Convention Center 211

8:00AM A19.00001 Transport in ultrathin gold films decorated with magnetic Gd atoms — MicOl AlemAni, erIck HelCren, Addison HuGeI, frAncEs HeIlman, Physics Department, University of California, Berkeley, 366 Le Conte, Berkeley, CA, 94720 — We have performed four-probe transport measurements of ultrathin Au films decorated with Gd ad-atoms. The samples were prepared by quench condensation, i.e., sequential evaporation on a cryogenically cooled substrate under UHV conditions while monitoring the film thickness and resistance. Electrically continuous Au films at thickness of about 2 mono-layers of material are grown on an amorphous Ge wetting layer. The quench condensation method provides a sensitive control on the sample growth process, allowing us to tune the morphological and electrical configuration of the system. The ultrathin gold films develop from an insulating to a metallic state as a function of film thickness. The temperature dependence of the Au conductivity for different thickness is studied. It evolves from hopping transport for the insulating films, to a ln T dependence for thicker films. For gold films in the insulating regime we found a decreasing resistance by adding Gd. This is in agreement with a decreasing tunneling barrier height between metallic atoms. The Gd magnetic moments are randomly oriented for isolated atoms. This magnetic disorder leads to scattering of the charge carriers and a reduced conductivity compared to nonmagnetic materials.
8:12AM A19.00002 From Order to Disorder and Back: Co on Narrow Stepped Cu, NADER ZAKI, DENIS POTAPENKO, RICHARD OSGOOD, JR., Columbia University, PETER JOHNSON, Brookhaven National Lab — Bimetallic surface systems allow a ready template to explore the compositional dependence of surface phases. When these systems involve a vicinal substrate, the surface also becomes a template for nanoscale-phase formations. In this regard, we examine the bimetallic system of Co on Cu(775), due the wide-spread interest in the magnetic phenomena of the related Co/Cu(111). We present an STM imaging study of this surface to show that it is possible to observe self-assembly of reduced-dimension quantum structures. These observations show that a rich set of bimetallic phase transitions as a function of coverage – moving from wires at low coverage to step-induced ordered islands at high coverage. At coverage of less than 0.1ML, we observe growth of sharp, straight 2-atom-wide Co wires; topographic measurements suggest an interesting interpretation of recent DFT computations on such a system. Increasing coverage causes a marked change of the step spacing and causes the surface to be covered with an ordered array of 2-D islands beyond a critical deposition amount. Thus, as coverage increases, the Cu step structure evolves from straight ordered step edges to concave-shaped edges and then from disordered to ordered islands.

8:24AM A19.00003 Electron charge and spin pairing (pseudo)gaps and Nagaoka instabilities in nanoclusters, ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University Los Angeles, GAYNATH FERNANDO, TUN WANG, KALUM PALANDAGE, Department of Physics, University of Connecticut, JIM DAVENPORT, Computational Science Center, Brookhaven National Laboratory — The electron pairings, phase separation and magnetism in various frustrated Hubbard clusters are studied exactly with emphasis on tetrahedron and octahedron under doping, magnetic field and temperature. Small clusters yield intriguing insight into charge spin separation and invoked thermal condensation of electron charge and spin in more than one bosonic mode. The spin saturated phase in so called Nagaoka state is found equivalent to ferromagnetic Mott-Hubbard like insulator with (negative) spin pairing gap, while non maximum spin ground state is of BCS-like metallic origin with equal charge (negative) and spin (positive) pairing gaps. The calculated phase diagrams resemble a number of inhomogeneous coherent and incoherent paired phases in high $T_c$ cuprates, fullerene molecules, Co and Nb nanoparticles.

8:36AM A19.00004 Superconductivity of Ultra-thin Pb films on Semiconductor Substrates: A Scanning Tunneling Microscopy/Spectroscopy Study, SHENGYONG QIN, JUNGDAE KIM, ALEXANDER AKO KHAJE-ToORIANS, CHIH-KANG SHIH, University of Texas at Austin — Ultra-thin Pb films on semiconductor substrates have exhibited many intriguing phenomena manifested by the quantum confinement of electronic states. Quantum confinement has been a topic of interest for many years. Recently, it was shown that quantum confinements also play an interesting role on superconductivity. Oscillations of superconductivity gap and $T_c$ as a function of film thickness have been observed in Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting confinement also plays an interesting role on superconductivity. Oscillations of superconductivity gap and $T_c$ as a function of film thickness have been observed in Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. By using a different surface template, namely Pb/Si(111) and Pb/Ge(111) systems. Moreover, it is found that the superconductivity remains very robust even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. 

8:48AM A19.00005 Magnetic field dependence of Interface Superconductivity in LSCO/LCO bilayers, SCOTT RIGGS, MagLab/FSU, FEDOR BALAKIREV, ALBERT MIGLIORI, MagLab/LANL, GREG BOEBINGER, MagLab/FSU, GENA LOGVENOV, ANTHONY BOLLINGER, ADRIAN GOZAR, IVAN BOZOVIC, BNL, LANL COLLABORATION, BNL COLLABORATION — Interface superconductivity (IS) with a high $T_c$ has been discovered recently in bi-layer films consisting of a thin layer of $La_1.55Sr_{0.5}CuO_4$ (overdoped and metallic but not superconducting) covered with a thin layer of $La_2CuO_4$ (undoped, insulating, and antiferromagnetic) grown by molecular beam epitaxy (MBE). Here we report on a study of magneto-transport properties in such IS systems. By measuring the magnetic-field dependence of in-plane longitudinal and Hall resistivities we find the temperature dependence of the upper critical field ($H_{c2}$). Other findings and inferences on the nature of IS and $T_c$ enhancement will be discussed as well.

9:00AM A19.00006 Separation of the strain and finite size effect on the ferromagnetic properties of $La_{0.5}Sr_{0.5}CoO_3$ thin films, CHANGKUN XIE, JOSEPH BUDNICK, BARRETT WELLS, Department of Physics, University of Connecticut, Storrs, CT 06269-3046, JOSEPH WOICIK, National Institute of Standards and Technology, Gaithersburg, Maryland 20899 — The ferromagnetic properties of epitaxial $La_{0.5}Sr_{0.5}CoO_3$ thin films have been studied. The magnetic transition is affected by both strain and finite thickness. We have used a series of films of different thickness and on different substrates in order to quantitatively determine the change in Curie temperature contributed by each effect. The phase diagram of $T_c$ versus in-plane strain suggests that the ferromagnetic transition temperature is suppressed by tensile strain and enhanced by compressive strain. The general method of separating strain and finite thickness effects should be applicable to any ordering phase transition in thin films. A leading theory for the ferromagnetism in $La_{0.5}Sr_{0.5}CoO_3$ is the double exchange mechanism. This model relies upon Co-O-Co electron hopping so that a strong dependence on bond length is expected. Our recent EXAFS results will examine whether the double exchange mechanism quantitatively predicts the strain dependence we have measured.

9:12AM A19.00007 Giant Magnetoelastic Coupling in Asymmetric Ferromagnet-Ferroelectric-Metal Trilayers: Toward Electric Control of Magnetization, TIANYI CAI, University of Texas at Austin, SHENG JU, Department of Physics, Suzhou University, Suzhou, 215006, China, JUNREN SHI, ENGE WANG, Institute of Physics and ICQS, Chinese Academy of Sciences, Beijing 100080, China, ZHENYA LI, Department of Physics, Suzhou University, Suzhou 215006, China, QIAN NIU, University of Texas at Austin — By examining electron screening at the surface of ferromagnetic metals and semiconductors, we propose an asymmetric ferromagnet-ferroelectric-metal trilayer to realize giant magnetoelastic effect. The origin is the strengthened accumulation of spin-polarized screening electrons at the ferromagnet-ferroelectric interface. Including the electrostatic energy from such spin-polarized charges in the Laudau-Devilbiss free energy for ferroelectrics, a magnetoelastic coupling term $\chi P^2M^2$ is derived, and consequently an electric control of magnetization hysteresis is observed. The dependence of $\chi$ as well as the ME effect on the choice of materials is discussed for some real ferromagnets.

9:24AM A19.00008 Room temperature ferromagnetism in as-deposited and post-annealed Co-doped ZnO films, XIAO-HONG XU, XIAO-LI LI, Shansi Normal University, China, G.A. GEHRING, University of Sheffield, UK — The Co-doped ZnO thin films were prepared on c-cut sapphire substrates by magnetron co-sputtering, and then annealed at various temperatures in vacuum. Magnetic measurements indicate that all the films are ferromagnetic at room temperature and the magnetization of the annealed $ZnO:8.8$CoO$_{12}$O films is increased about one order of magnitude in comparison with the corresponding as-deposited one. Both X-ray diffraction and TEM results show that there are not any Co and Co oxides secondary phases. Optical spectrometry indicates that Co$^{2+}$ enters the tetrahedral sites of the wurtzite structure of ZnO host and substitutes for Zn$^{2+}$.

1Supported by grant Nos. 10574085 and 60776008 of NSF of China, NCET-07-0527 of China and the Leverhulme Trust of UK.

2Supported by grant Nos. 10574085 and 60776008 of NSF of China, NCET-07-0527 of China and the Leverhulme Trust of UK.
9:36AM A19.00009 Ferromagnetic $\text{Mn}_3\text{Ga}$ On Wurtzite GaN: Initial Stages Of Growth By Molecular Beam Epitaxy, KANGKANG WANG, ABHIJIT CHINCHORE, EORDONG LU, WENZHI LIN, JEONGHIM PAK, ARTHUR R. SMITH, Nanoscience and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, OH 45701 — Ferromagnetic (FM) metal/wide-bandgap bilayers are of great interest due to their potential for novel spintronics applications, such as blue and ultra-violet light-emitting diodes. It has been reported that $\text{Mn}_3\text{Ga}$, a promising FM alloy, can be grown epitaxially on top of w-GaN(0001) with controllable magnetism via controlling of the Mn:Ga flux ratio. Here we report studies on the initial stages of growth of MnGa on w-GaN. Growth experiments were carried out in a UHV chamber using molecular beam epitaxy with rf (N$_2$)-plasma, on both N- and Ga-polar substrates. Reflection high-energy electron diffraction (RHEED) data suggest that at the initial stages of growth, the surface structures depend on the substrate polarity. This may be due to the structural differences between the N-polar and the Ga-polar GaN surfaces. Stoichiometry dependence of initial stages of growth is also being investigated. This work has been supported by DOE (Grant No.DE-FG02-06ER46317) and NSF (Grant No.0304314). Equipment support from ONR is also acknowledged. [1] S.A.Wolf et al, Science 294, 1488 (2001) [2] E.Lu et al, Phys.Rev.Lett. 97, 146101 (2006)

9:48AM A19.00010 Molecular Beam Epitaxial Growth of Iron Nitrides on Zinc-Blende Gallium Nitride (001), JEONGHIM PAK, WENZHI LIN, ABHIJIT CHINCHORE, KANGKANG WANG, ARTHUR R. SMITH, Nanoscience and Quantum Phenomena Institute, Department of Physics & Astronomy, Ohio University, Athens, OH 45701 — Iron nitrides are attractive materials for their high magnetic moments, corrosion, and oxidation resistance. We present the successful epitaxial growth of iron nitride on zinc-blende gallium nitride (c-GaN) in order to develop a novel magnetic transition metal nitride/semiconductor system. First, GaN is grown on magnesium oxide (MgO) substrates having (001) orientation using rf N$_2$-plasma molecular beam epitaxy. Then we grow FeN at substrate temperature of $\sim$ 210 °C up to a thickness of $\sim$ 10.5 nm. In-situ reflection high-energy electron diffraction (RHEED) is used to monitor the surface during growth. Initial results suggest that the epitaxial relationship is FeN[001] $\parallel$ GaN[001] and FeN[100] $\parallel$ GaN[100]. Work in progress is to investigate the surface using in-situ scanning tunneling microscopy (STM) to reveal the surface structure at atomic scale, as well as to explore more Fe-rich magnetic phases.

10:00AM A19.00011 Synthesis of $\text{Co}_{1-x}\text{Fe}_{2x}\text{O}_4$: Towards Spin Polarized Ferrites, JARRETT MOYER, HUI-QIONG WANG, Department of Applied Physics, CRISP, Yale University, CARLOS VAZ, CRISP, Yale University, VICTOR HENRICH, Department of Applied Physics, CRISP, Yale University — Ferrites are promising materials for spintronic devices, since they are predicted to exhibit high spin polarizations [1]. Thin-film cobalt ferrite (CoFe$_2$O$_4$) has a large saturation magnetization and magnetic coercivity, but is insulating [2]. In this work, epitaxial $\text{Co}_{1-x}\text{Fe}_{2x}\text{O}_4$ thin films are grown by MBE on Fe$_3$O$_4$(001) and MgO(001), where a fraction of the Co$^{2+}$ ions are replaced with Fe$^{3+}$. LEED, RHEED and XRD confirm the crystal structure. Stoichiometry and cation valence states are ascertained by XPS, and the electronic structure near the Fermi level is determined by UPS. We show, that by varying the stoichiometry of $\text{Co}_{1-x}\text{Fe}_{2x}\text{O}_4$, we can tailor its electronic properties, which may lead to a conductive, spin polarized ferrite. [1] J. Cibert, et al., C.R. Physique 6 (2005) 977. [2] W. Huang, et al., J. Crystal Growth 300 (2007) 426.

1 This research is primarily supported by NSF Grant MRSEC DMR-0520405

10:12AM A19.00012 A surface-driven route to novel magnetic structures: Manganese on Si(100), PETRA REINKE, HUI LIU, CHRISTOPHER NOLPH, University of Virginia — The combination of Silicon with an element with a large magnetic moment such as Manganese is highly desirable for the development of novel spintronics devices. We present a study on the surface-driven synthesis of Mn-nanostuctures on the Si(100) (2x1) surface using STM and photoelectron spectroscopy. The Si-surface functions as a template and monatomic Mn-nanowires are formed, which always run perpendicular to the Si-dimer rows. Their length and spatial distribution is used to derive a model for the wire formation. The bonding of Mn to the Si, which is decisive for the resultant magnetic properties, are presented. The transition to a silicide is kinetically hindered and controlled by the Si-mobility. In the next step a Ge-overlayer is deposited, and analyzed with voltage dependent STM. In the low-adatom-mobility regime the Ge-growth is unperturbed by the presence of Mn, and the Mn-nanostructure is preserved and embedded.

3 The authors gratefully acknowledge the support of this work by the Nanoelectronics Research Initiative (NRI) in conjunction with NSF

10:24AM A19.00013 High-resolution ARPES studies of atomically uniform Pb films on Si(111), SHAOULONG HE, MASASHI ARITA, MASAHIRO SAWADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan, SHAN QIAO, Lawrence Berkeley National Laboratory, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, Hiroshima University, Hiroshima 739-0046, Japan. Of great interests both in basic research and in potential applications. Atomically uniform metal thin films on semiconductor substrate are the simplest quasi-2D electron systems, which demonstrate quantum confinement and form the quantum well states (QWS). Recently, atomically uniform Pb films on Si(111) have demonstrated novel properties induced by the quantum size effects. We have manufactured atomically uniform Pb films on Si(111)-7x7 surface. The dependence of the Pb films band structures on thickness has been studied by high-resolution angle-resolved photomission spectroscopy (ARPES). In addition, we have investigated the superconductivity properties in such a quasi-2D electron systems by measuring the ARPES below superconducting transition temperature.

10:36AM A19.00014 Unusual Hall effect due to carrier delocalization, XIAOHANG ZHANG, S. VON MOLNAR, P. XIONG, Florida State University, Z. FISK, University of California at Irvine — The spin polarization of EuB$_6$ crystals has been measured using Andreev reflection spectroscopy. The conductance spectra of the EuB$_6$/Pb junctions are well-described by the spin-polarized BTK model, which yields a spin polarization of about 56%. The results demonstrate that ferromagnetic EuB$_6$ is not half-metallic. Further analyses of the Hall effect and magnetoresistance indicate a semi-metallic band structure with complete spin polarization for the hole band only. The values and the spread of the measured spin polarization is quantitatively consistent with Fermi surface determined by quantum oscillation measurements and carrier densities obtained from standard two-band model fits to the low temperature magnetoresistivity and Hall resistivity. This work was supported by a FSU Research Foundation PEG, NSF DM 0710492 and 0503360 grants. 1. R. Goodrich et al., PRB 58, 14896 (1998); M. Aronson et al., PRB 59, 4720 (1999).

10:48AM A19.00015 Spin-dependent band structure of the ferromagnetic semimetal EuB$_6$, PENG XIONG, X. ZHANG, S. VON MOLNAR, Florida State University, Z. FISK, University of California at Irvine — The spin polarization of EuB$_6$ crystals has been measured using Andreev reflection spectroscopy. The conductance spectra of the EuB$_6$/Pb junctions are well-described by the spin-polarized BTK model, which yields a spin polarization of about 56%. The results demonstrate that ferromagnetic EuB$_6$ is not half-metallic. Further analyses of the Hall effect and magnetoresistance indicate a semi-metallic band structure with complete spin polarization for the hole band only. The values and the spread of the measured spin polarization is quantitatively consistent with Fermi surface determined by quantum oscillation measurements and carrier densities obtained from standard two-band model fits to the low temperature magnetoresistivity and Hall resistivity. This work was supported by a FSU Research Foundation PEG, NSF DM 0710492 and 0503360 grants. 1. R. Goodrich et al., PRB 58, 14896 (1998); M. Aronson et al., PRB 59, 4720 (1999).
Monday, March 10, 2008 8:00AM - 10:48AM –
Session A20 DMP: Focus Session: Quantum Dots and Semiconductor Surface Nanostructures
Morial Convention Center 212

8:00AM A20.00001 Phase-field modeling of solute precipitation and dissolution at solid-fluid interface. ZHUIIE XU, PAUL MEAKIN, Idaho National Laboratory — Phase phase-field methods have been developed to simulate a variety of processes in which interface dynamics play a critical role. The mathematical formulation of a phase field approach to the dynamics of liquid solid interfaces that evolve due to precipitation and/or dissolution will be presented. For the purpose of illustration, and comparison with other methods, phase field simulations have been carried out assuming first order reaction dissolution/prediction) kinetics. In contrast to solidification processes controlled by a temperature field that is continuous at the solid/liquid interface, with a discontinuous temperature gradient, precipitation/dissolution is controlled by a solute concentration field that is discontinuous at the solid/liquid interface. The sharp-interface asymptotic analysis of the phase-field equations for solidification by Karma and Rappel [Phys. Rev. E57 (1998) 4342] have been extended to demonstrate that the phase-field equations converge to the proper sharp-interface limit for the precipitation/dissolution problem. The mathematical model has been validated for a one-dimensional precipitation/dissolution problem by comparison with the analytical solutions of the free-boundary problem.

8:12AM A20.00002 Island Size Scaling and Evolution during Strained Film Epitaxy. ZHI-FENG HUANG, Department of Physics and Astronomy, Wayne State University; KEN ELDER, Department of Physics, Oakland University — Strained film growth often gives rise to the self assembly of nanostructures such as quantum dots or islands. While there has been and continues to be much interest in such behavior the fundamental mechanisms that determine the precise morphologies remain unclear. In this work the phase field crystal model, which incorporates the atomic length and diffusive time scales, and the corresponding amplitude equations are used to examine this phenomenon. Direct numerical simulations of the model and linear stability analysis of the amplitude equations are presented. The results predict that the average island size is inversely proportional to the strain. This result is consistent with recent experiments on SiGe, but inconsistent with the predictions of classic continuum elasticity theory (or the Asaro-Tiller-Grinfeld instability). Basic mechanisms identified in our study, which are associated with the crystalline nature but absent in all continuum approaches, are discussed.

8:24AM A20.00003 Optimal Capping Layer Thickness for Stacked Quantum Dots. XIAOBIN NIU, Department of Material Sciences and Engineering, UCLA, Los Angeles, CA 90095, CHRISTIAN RATSCH, Department of Mathematics/Institute for Pure and Applied Mathematics, UCLA, Los Angeles, CA 90095, YOUNG-JU LEE, Department of Mathematics, UCLA, Los Angeles, CA 90095, RUSSEL CAFLISCH, Department of Mathematics/Department of Material Sciences and Engineering, UCLA, Los Angeles, CA 90095 — We study the effect of strain on the vertical and lateral self-organization of nanoscale patterns and stacked quantum dots during epitaxial growth. The computational approach is based on the level set method in combination with an atomic strain code. Strain changes the energetics of microscopic parameters during growth, and thus determines the nucleation sites and the growth of islands and dots. Our results show that strain can lead to vertical alignment as well as lateral organization. Moreover, our simulations suggest that there is an optimal thickness of the capping layer to get the best alignment and most uniform size distribution of stacked quantum dots.

8:36AM A20.00004 Modeling the complex evolution of self-assembled quantum dots. JERRY TERSOFF, IBM T.J. Watson Research Center — In heteroepitaxy, misfit strain often leads to spontaneous formation of islands. Such islands have attracted great interest as “self-assembled quantum dots”. The growth of these quantum dots is remarkably rich, exhibiting alloy intermixing, island coarsening, trench formation, and even spontaneous lateral motion of islands. Islands also interact with topographic features on the substrate, providing a means for controlling the position of quantum dots. The diverse experimental observations provide an ideal opportunity to test and extend our theoretical understanding of growth at the nanoscale. We find that much of the complexity arises because there is a strong thermodynamic driving force for intermixing (to increase entropy and reduce strain energy) as well as for morphological evolution (to reduce strain energy); but this evolution must occur under the kinetic constraint of diffusion occurring only at the surface. Simulations of such constrained evolution directly reproduce many of the observed phenomena [Y. Tu and J. Tersoff, Phys. Phys. Lett. 98, 096103 (2007)].

3 Work done in collaboration with Yuhai Tu

9:12AM A20.00005 Effect of Elastic Inhomogeneity and Anisotropy on the Order of Epitaxial Self-Assembled Quantum Dots. CHANDAN KUMAR, LAWRENCE FRIEDMAN, Penn State University — Growth of epitaxial self-assembled semiconductor quantum dots (SAQDs) is of particular interest in the development of quantum dot based devices such as quantum computing architectures, laser diodes, and other optoelectronic devices. The ordering of these SAQDs is critical for the development of these devices. Understanding what factors the order of these SAQDs depend on, is important for guiding both experiments and simulations. Most theoretical and numerical models approximate the film substrate system as a semi-infinite solid. Although models based on such an approximation have been able to predict some general behaviour in confirmation with the experimental results, predictions about a quantitative measure would be less approximate if the models could incorporate elastic inhomogeneity. The presented linear stochastic model for SAQD growth incorporates elastic inhomogeneity and anisotropy along with stochastic surface diffusion to produce a more refined quantitative model for SAQD order formation. For the Ge/Si film-substrate system it is found that at the critical film height such an approximation could lead to an error of ~12% in the estimation of average spacing between SAQDs and an error of ~24% in the estimation of number of correlated dots for small height fluctuations.

9:24AM A20.00006 Composition Maps in Strained Alloy Quantum Dots. NIKHIL MEDHEKAR, VISH-WANATH HEGADEKATTE, VIVEK SHENOY, Brown University — Knowledge of composition profiles within self-assembled SiGe and InGaAs quantum dots is critical for applications in optoelectronic and memory devices as variations in composition at the nanoscale can substantially influence their electronic properties. Obtaining the quantitative description of composition profiles in the quantum dot is a challenging task due to the coupling between composition variations, shape of the quantum dots and long-range elastic interactions. In this talk, we present an efficient scheme that combines the finite element analysis with an optimization scheme based on a quadratic programming method to determine equilibrium profiles in strained quantum dots. Composition profiles are found to strongly depend on the shape of the quantum dots, as strain relaxation in dots with steeper sidewalls allows for segregation of the larger alloy component in the regions near the apex. Based on these observations, we have developed a phase diagram that shows the degree of segregation of the alloy components in the phase space spanned by the temperature (which governs chemical mixing) and the shape of the dot. Further, we find that the segregation of the alloy components can substantially reduce the critical dot size for the transition between the shapes with different facets.
9:36AM A20.00007 An Accelerated Molecular Dynamics Study of the GaAs (001) $\beta 2(2\times4)$ Reconstruction. MARIA MIGNOGNA, KRISTEN FICTHTHORN, Penn State University — The GaAs (001) $\beta 2(2\times4)$ reconstruction is the most commonly used substrate for growth in GaAs homoepitaxy by molecular beam epitaxy. While the atomic positions of the $\beta 2(2\times4)$ unit cell have been determined, reflection high energy electron diffraction and scanning tunneling microscopy images show long range disorder on this surface[1]. It is hypothesized that domains of anti-phase $\beta 2(2\times4)$ unit cells can be created by vacancies or As dimer shifts. Accelerated molecular dynamics (MD) allows us to examine atomic scale processes that can lead to this disorder. We have developed an adaptive accelerated MD scheme based on the bond boost method of Miron and Fichthorn[2]. The adaptive method is suitable for the rough energy landscape presented by GaAs (001). In the adaptive method, both the length thresholds for determining transition states and the magnitude of the boost are calculated on the fly. We are able to extend the physical timescale of the simulation by several orders of magnitude. We see events that lead to small domains of As dimers shifting. By simulating RHEED images of the surface, we link the disorder to experiment. [1] D.W. Pashley, J.H. Neave, B.A. Joyce, Surf. Sci., 582, 189 (2005) [2] R.A Miron, K.A. Fichthorn, J. Chem. Phys., 119, 6210 (2003)

9:48AM A20.00008 Strain and Piezoelectric Effects on the Electronic Structure of Coupled In$_{x}$Ga$_{1-x}$As/GaAs Self-Assembled Quantum Dots. USMAN MUHAMMAD, Purdue University, SHAIKH AHMED, Southern Illinois University Carbondale, GERHARD KLIMECK, Purdue University — In$_{x}$Ga$_{1-x}$As/GaAs coupled quantum dot systems have gained much attention for optical and quantum computing applications. Due to strain, originating from the assembly of lattice mismatched semiconductors, the quantum dot arrays tend to grow in the vertical direction. These vertically stacked dots are strongly coupled through the strain field, which is atomically inhomogeneous and penetrates deep into the GaAs buffer layer surrounding the dots. Crystal symmetry and atomistic details of interfaces are extremely important in such systems. Also piezoelectric fields must be taken into account to properly model the experimentally observed symmetry breaking and the introduction of a global shift in the energy spectra of the system. In this work, we present a detailed description of strain and piezoelectric potential effects on the electronic structure of closely coupled identical and non-identical quantum dot systems using spd$^{s*}$ nearest neighbor empirical tight binding model. We show that strain causes strong mixing of s- and p- electron energy levels in strongly coupled quantum dot, splits heavy hole and light hole bands and even reverses their order within dots.

10:00AM A20.00009 Structure competition in growth of In island on Si111 from first-principles calculations. CAI-ZHUANG WANG, MIN JI, J. CHEN, M. HUPALO, M.C. TRINGIDES, K.M. HO, Ames Laboratory US-DOE and Department of Physics, Iowa State University, Ames, IA 50011, USA — We have carried out first principles calculations to understand the growth of indium island on Si111 substrate which have been observed to have an interesting FCC and BCT structure competition. Our calculations show that quantum size effect (QSE) plays an important role in different island structure formation. Furthermore, the interplane energy between In and Si substrate also controls the relative stability of different island structures.

10:12AM A20.00010 Thermodynamic potentials in closed and open nanocrystalline systems: Si-Ge islands on Si(001). MARINA S. LEITE, Brazilian Synchrotron Light Source, Instituto de Fisica Gleb Wataghin - UNICAMP, ANGELO MALACHIAS, Max-Planck Institute for Solid State Research, STEFAN W. KYCIA, University of Guelph, TED I. KAMINS, R. STANLEY WILLIAMS, Hewlett-Packard Laboratories, GILBERTO MEDEIROS-RIBEIRO, Hewlett-Packard Laboratories, Brazilian Synchrotron Light Source — The driving forces for alloying in Si-Ge epitaxial nanocrystalline islands were quantified experimentally. Grazing Incidence X-Ray Diffraction (GIXRD) experiments were performed to map the composition and the strain distribution within the Si-Ge:Si(001) islands, permitting the evaluation of the relevant thermodynamic potentials for alloying. For the closed system the elastic strain energy increased, which was more than compensated by the increase in the local mixing entropy [2]. In contrast, for the open system, the elastic energy decreased and the mixing entropy increased, driven by the intermixing originated from the relevant of Si from the reservoir. For both systems, the evolution of the composition leads to a lowering of the Gibbs free energy. The results were in full agreement with a theoretical prediction of the optimum concentration for epitaxial islands. [1] M. S. Leite et al, Phys. Rev. Lett. 98, 156501 (2007). [2] G. Medeiros-Ribeiro et al, Nano Lett. 7, 223 (2007).

10:24AM A20.00011 Characterization of MBE grown PbSe Quantum Dots. NATHANIEL BECKER, DUSTN KLEIN, TIM KIDD, Univ of Northern Iowa — Lead selenide (PhSe) has been shown to be an excellent candidate for solar cell research due to its ability to allow the possibility for multiple electronic carrier production by absorption of a single photon. These quantum dots (QDs) were created using molecular beam epitaxy (MBE) to evaporate PbSe onto clean and modified silicon and germanium substrates. Control of lattice strain was achieved by the deposition of buffer layers onto clean Si(111)in ultra-high vacuum. The MBE technique allows for structural control at the atomic level. We have investigated the samples using Auger spectroscopy, scanning probe and scanning electron microscopy to determine their suitability for solar cell applications. Specifically, we examined the structural properties of the system. In this work, we present a detailed description of strain and piezoelectric potential effects on the electronic structure of closely coupled identical and non-identical quantum dot systems using spd$^{s*}$ nearest neighbor empirical tight binding model. We show that strain causes strong mixing of s- and p- electron energy levels in strongly coupled quantum dot, splits heavy hole and light hole bands and even reverses their order within dots.

10:36AM A20.00012 Self Assembling Quantum Dot Aggregates in Liquid Crystal Matrices. CHRISTOPHER FERRI, M. GALLARDO, Y. VERMA, D. KELLEY, S. GHOSH, School of Natural Sciences, University of California, Merced CA 95343 — A system of colloidal quantum dots (QDs) embedded in a matrix of highly directional and ordered liquid crystal (LC) molecules at room temperature offers the novel potential of promoting controllable aggregation of the QDs. Photoluminescence (PL) of GaSe QDs embedded in a LC matrix, studied using a confocal-microscopy setup, shows considerable red-shift in the emission spectrum of the QD-LC composite. While bare QDs in solution emit at 485 nm, mixing with LC molecules results in an emission centered at 500 nm, system suggesting their aggregation into longer structures in the matrix. A high resolution two-dimensional spatial map of the PL on the sample provided evidence of the organization of QDs into these ordered domains. Application of in-plane electric fields further enhances the aggregation effect of the QDs and emission spectrum is red-shifted to around 525 nm. Furthermore, as the aligning electric field increases the degree of ordering of the liquid crystal molecules, the polarization ($P$) of the emission of the aggregated QDs rotates in step with that of the LCs' directionality. Unlike the disc-shaped GaSe QDs, investigations on LC and CdSe QD system failed to show such dramatic aggregation effects.

1NSF: IGERT grant DGE 9987589 and grant DMR 0514336

Work supported by ARO
8:00AM A21.00001 Self Assembly of Mixed-Valence Ionic Amphiphiles into Faceted Vesicles. MEGAN GREENFIELD, GRAZIANO VERNIZZI, LIAM PALMER, SAMUEL STUPP, MONICA OLVERA DE LA CRUZ. Northwestern University — We show that anionic and cationic amphiphiles of unequal charge can co-assemble into small faceted vesicles and we propose a theoretical model to explain the faceting behavior. The strong electrostatic interaction between the +3 and -1 head groups increases the Columbic cohesion energy of the amphiphiles and should favor the formation of a two-dimensional, flat ionic surface. The vesicle surface can form edges by breaking the ionic lattice, which can be visualized as faceted shapes. Our results demonstrate that a large charge imbalance between the cationic and anionic head groups of amphiphiles enables their coassembly into faceted vesicles. We anticipate this work to be a starting point for rationally designing new self-assembled supramolecular structures.

8:12AM A21.00002 Electrospinning Solutions of Associating Polymers – the Case of Stereocomplex PMMA. MATJIA CRNE, JUNG PARK, MOHAN SRINIVASARAO, Georgia Institute of Technology — A mixture of isotactic and syndiotactic PMMA polymers (also called a “stereocomplex PMMA”) forms a supramolecular helical structure, which is held together by non-covalent bonding. This association is thermoreversible and solvent-sensitive. If the concentration of stereocomplex PMMA is high enough, the solutions form thermoreversible physical gels. We have examined this influence through the process of electrospinning. In our work, we have used solutions of stereocomplex PMMA to study the effect of physical gelation interaction on the fiber morphology and compared it to the solutions of atactic PMMA of similar molecular weight. We have found that the stereocomplex PMMA solutions do not follow the same empirical rules that are applicable for linear polymers in solution. Instead, the concentration necessary for the production of smooth, continuous fibers is much lower. We ascribe this extraordinary behavior to the ability of these polymers to associate and form a network during the electrospinning process. The elasticity of the fluid jet thus rises and results in a more stable jet. The resulting fibers are interesting, as they have greater temperature stability than regular atactic PMMA. Therefore they have a bigger processing window for making composites with better mechanical properties.

8:24AM A21.00003 ABSTRACT WITHDRAWN

8:36AM A21.00004 Unique Properties of Reversibly Associating Polymer Networks1, MITCHELL ANTHAMATTEN, University of Rochester — Reversibly associating functional groups offer the polymer physicist with a new tool to develop stimuli-responsive polymers. Our focus has been to attach reversibly associating groups onto rubbery network polymers. Free radical copolymerization was used to synthesize a series of crosslinked poly(n-butylacrylate)s containing quadruple H-bonding ureidopyrimidinone (UPy) side-groups. Resulting elastomeric networks contain both covalent and dynamic non-covalent crosslinks, and this unique architecture is shown to affect viscoelastic behavior and mass-transport properties. Shape-memory effects are studied quantitatively using thermomechanical techniques. Experiments show how reversible interactions, such as hydrogen bonding, are capable of stabilizing mechanically strained states. Unlike conventional shape-memory polymers, these dynamic networks lack a well-defined shape recovery temperature. Instead, their shape recovery rate depends on temperature. To further study the dynamics and temperature dependence of mechanical relaxation, isothermal creep experiments and dynamic mechanical analysis were performed. Creep data, acquired at several different temperatures, are fit to a simple viscoelastic model. Fit viscosities exhibit Arrhenius-like temperature dependence with activation energies of ~90 kJ/mol, which is in rough agreement with H-bond dissociation barriers. Molecular transport through dynamic networks is studied using gravimetric sorption and dye-diffusion techniques. Diffusion depends on temperature, network architecture, solute size, and the interaction between the solute and the network. Membranes with high temperature-sensitive diffusion properties may be useful in applications such as transdermal drug delivery, microfluidics, or liquid chemical separation processes.

1Supported by NSF grant DMI-0423619

9:12AM A21.00005 Computer Simulations of Semi-flexible Polymer Chains. VENKAT PADMANABHAN, SANAT K. KUMAR, Columbia University, ARUN YETHIRAJ, University of Wisconsin — Monte Carlo Simulations are performed to obtain the isotropic-nematic (IN) transition in systems with semi-flexible polymer chains of different lengths. The chains are modeled as spherical beads that interact via a square-well potential. Bonded beads are connected by strings chosen so that bond length varies between 1.0σ and 1.05σ (where σ is the hard sphere diameter). The stiffness of the molecules is controlled via a potential between beads separated by two bonds; this potential restricts the distance between these beads to be between 2.0σ and 2.1σ. The vapor-liquid coexistence and isotropic-nematic (IN) coexistence curves are obtained using computer simulations. An IN transition is found for NΩ > 10. The density, at which the IN transition occurs, moves to higher values as NΩ is increased and then drops on further increase. This is analogous to the initial increase in the critical density for pure alkanes as the chain length is increased.

9:24AM A21.00006 Reversible Networks by Hydrogen Bonding of ABA Triblock Copolymers in an Ionic Liquid. TIMOTHY LODGE, University of Minnesota. ATSUSHI NORO, YUSHU MATSUSHITA, University of Nagoya — Ion gels, comprising a polymeric network solvated by an ionic liquid, are of great interest as, e.g., gate dielectrics in plastic electronics, polymer electrolytes with high ionic conductivity, actuators and artificial muscles, gas separation media, and sensors. We have explored the thermoreversible gelation of a model system containing poly(2-vinyl pyridine-b-ethyl acrylate-b-2-vinyl pyridine) (VEAV) triblocks dissolved in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [em][tfsi], with better mechanical properties.

9:36AM A21.00007 Examination of the Structure of Molten Hydrogen-Bonded Supramolecular Diblock Copolymers. KATHLEEN FELDMAN, MATTHEW KADE, CRAIG HAWKER, EDWARD KRAMER, UCSB — A new strategy for synthesizing low polydispersity polymers containing multiple hydrogen bonding (HBB) groups at one chain end capable of heterodimerization in both solution and the melt has been developed. Two well-known MHB systems were chosen for initial studies—2-ureido-4[1H]-pyrimidinone (UPy) and 1,8-diaminodiphenylhexidine (Nap), and ATRP initiators containing either UPy or Nap were synthesized. These initiators were shown to produce well-defined (meth)acrylic polymers with the desired HBB functionality present at the chain end. To characterize the effectiveness of the HBB interaction in the melt, blends were cast into films, annealed at various temperatures above Tg, then quenched and their structure analyzed by transmission electron microscopy (TEM) and differential scanning calorimetry (DSC). It was shown that the nature of the hydrogen bonding group(s) present in the blend has a significant effect on structure and thermal behavior, and in particular blends of UPy- and Nap-functional chains contain a significant fraction of “supramolecular diblock copolymers.”

9:48AM A21.00008 Thermoreversible bond formation in end-linking, difunctional polymer blends. RICHARD ELLIOTT, GLENN FREDRICKSON, Materials Research Laboratory, University of California, Santa Barbara — We investigate theoretically thermoreversible bond formation and phase transitions in a system composed of linear, end-linking, difunctional polymers. In this melt, two distinct species of equal-length links assemble into chains of varying sequences and polymerization depending on the affinities of binding between the blocks. Several limits, such as that of purely heterogeneous bonding which forms chains of alternating block sequences, are explored. Interactions between dissimilar segments are described with the Flory-Huggins contact potential and a mean-field approach is employed to investigate the effects of prevailing bond and the onset of meso-scale ordering.
10:00AM A21.00009 Inter- and Intra-Molecular Interactions of Associative Polymers in Solution, M. WEI, R. DAVID, JULIE KORNFIELD, Caltech — Model polymers with matched backbone length are used to examine the effects of degree of functionalization and type of interaction (self-associating or donor-acceptor) on shear and extensional rheology of associative polymer solutions. Series of polymers were prepared by functionalization of 500 and 1300 kg/mol polybutadiene chains with carboxylic acid side groups (A stickers, self-associating) and tertiary amine side groups (N stickers, forming strong hydrogen donor-acceptor interactions with A stickers). We found that stickers drive phase separation at extents of functionalization as low as 0.5 mol%. Intramolecular associations dominated the behavior of A-functionalized chains even at semi-dilute concentrations, leading to chain collapse and reduced shear and extensional viscosities. Finally, we found that intermolecular interactions were much more favorable for dilute mixtures of A-functionalized and N-functionalized chains (as evidenced by increased zero-shear viscosity and by the formation of large aggregates), but that associations still reduced solution elasticity and extensional viscosity in elongational flow.

10:12AM A21.00010 Molecular Dynamics Simulation of Polyelectrolyte Brushes: From Hemispherical Micelles to Maze-like Aggregates, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science, University of Connecticut — We present results of the molecular dynamics simulations of the effects of solvent quality, strength of the electrostatic interactions, chain degree of polymerization and grafting density on the conformations of planar polyelectrolyte brushes in salt-free solutions. The polyelectrolyte brush could form: (1) hemispherical micelle aggregates, (2) vertically oriented cylindrical micelles, (3) maze-like aggregate structures, or (4) thin polymeric layer uniformly covering the substrate. These different brush structures appear as a result of the fine interplay between electrostatic and monomer-monomer attractive interactions. The brush thickness depends nonmonotonically on the value of the Bjerrum length. This nonmonotonic dependence is due to counterion condensing inside the brush.

10:24AM A21.00011 Effect of Hydrogen-Bonding Junctions on Microphase Separation in Block Copolymers, GREG STONE, University of California Berkeley, JIM HEDRICK, FREDRIK NEDERBERG, IBM Almaden Research Facility, NITASH BALSARA, University of California Berkeley, CPIMA COLLABORATION — The morphology of poly(styrene-block-trimethylene carbonate) (PS-PTMC) copolymers with and without thiourea groups at the junction between the blocks was studied by a combination of small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). The thiourea groups are known to exhibit inter-molecular hydrogen bonding. We demonstrate that the presence of thiourea groups results in increased segregation between PS and PTMC blocks. We focus on symmetric systems with total molecular weights in the 5 kg/mol range. In conventional block copolymers without hydrogen bonding groups it is difficult to obtain strong segregation in low molecular weight systems because the product chi*N controls segregation (chi is the Flory-Huggins interaction parameter and N is the number of monomers per chain). The incorporation of hydrogen bonding groups may provide a route for the generation of patterns with small, sharply defined features using block copolymers.

10:36AM A21.00012 Relating Chain Structure to Physical Properties of Branched Polymers, RAMNATH RAMACHANDRAN, GREGORY BEÀUCAGE, AMIT S. KULKARNI, University of Cincinnati, VASSILIOS GAlIATsATOS, DOUGLAS C. MC-FADDIN, LyondellBasell Industries — We investigated linear and branched polyethylene (PE) using small-angle neutron scattering (SANS). The experiments were conducted on dilute solutions of PE in deuterated p-xylene. A variety of structural information such as fractal dimension (d(1)), connectivity dimension (c), minimum path dimension (d(min)), long chain branch fraction (phi_d), radius of gyration (R_g) and persistence length (l_p) were obtained. Such information presents a qualitative and quantitative assessment of branching in polymers. Theoretical models such as ‘binary contacts per pervaded volume’ model were employed to correlate the structural information of the polymer to its entanglement molecular weight (M_e). M_e was used to predict physical properties such as plateau modulus (G_0) and zero-shear viscosity (eta_0). We relate physical properties of branched polymers to their structural properties. Beaucage G. Physical Review E 70,031401 (2004) *Colby et al. Macromolecules 25, p.996 (1992)

1Work was supported by LyondellBasell Industries. Results shown in this report are derived from work performed at Argonne National Laboratory. Argonne is operated by UChicago Argonne, LLC, for the U.S. Department of Energy under contract DE-AC02-06CH11357

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A22 DPOLY: Focus Session: Hybrid Organic-Inorganic Nanomaterials I: Patterning and Self Assembly Morial Convention Center 214

8:00AM A22.00001 Connecting quantum dots and bionanoparticles in hybrid nanoscale ultrathin films, RAVISUBHASH TANGIRALA, YUNXIA HU, QINGLING ZHANG, JINBO HE, THOMAS RUSSELL, TODD EMRICK, University of Massachusetts, Amherst — Aldehyde-functionalized CdSe quantum dots and nanorods, and horse spleen ferritin bionanoparticles, were co-assembled at an oil-water interface. Reaction of the aldehydes with the surface-available amines on the ferritin particles enabled cross-linking at the interface, converting the assembled nanoparticles into robust ultra-thin films. The cross-linked capsules and sheets thus made by aldehyde-amine conjugation could be disrupted by addition of acid. Reductive amination chemistry could be performed to convert these degradable capsules and sheets into structures with irreversible cross-linking. Fluorescence confocal microscopy, scanning force microscopy and pendant drop tensiometry were used to characterize these hybrid nanoparticle-based materials, and transmission electron microscopy (TEM) confirmed the presence of both the synthetic and naturally derived nanoparticles.

8:12AM A22.00002 Janus Au Nanoparticle Patterning via Polymer Single Crystals, CHRISTOPHER LI, BING LI, Drexel University — Gold nanoparticles (AuNPs) possess remarkable electrical and optical properties coupled with good chemical stability. Thus, they have wide potential applications in fabrication of advanced optical and electronic devices. In order to efficiently transfer their outstanding properties from nano- to micro-scale, patterned AuNPs are desired. Here, we report a novel method using polymer single crystals as substrates to pattern AuNPs. By using thiol-terminated polyethylene oxide (HS-PEO) as the substrate, we were able to assemble AuNPs into different patterns on the PEO single crystals. Furthermore, these AuNPs are asymmetrically functionalized (Janus NPs). A variety of shapes including chains and sheets were formed, and the size and areal density of the AuNP assemblies can be controlled through the AuNP adding time and the ratio between AuNPs and polymer single crystals, respectively. Because of the asymmetrical nature of the AuNPs, the resultant chains and sheets are both asymmetric (Janus chains and Janus sheets), which could lead to a variety of interesting optic properties. We anticipate that our approach would provide a facile means to pattern AuNPs, and it could be extended to other metal and semiconductor NPs.
8:24AM A22.00003 Organic-Inorganic Nanocomposites via Directly Grafiting Conjugated Polymers onto Quantum Dots, ZHIQUN LIN, Iowa State University, JUN XU, JUN WANG, MIKE MITCHELL, PRASUN MUKHERJEE, MALIKA JEFFRIES-EL, JACOB W. PETRICH, Iowa State University — Nanocomposites of poly(3-hexylthiophene)-cadmium selenide (P3HT-Cds) were synthesized by directly grafting vinyl terminated P3HT onto [4-(bromophenyl)methyl]diocylphosphine oxide (DOPO-Br)-functionalized CdSe quantum dot (QD) surfaces via a mild palladium-catalyzed Heck coupling, thereby dispensing with the need for ligand exchange chemistry. The resulting P3HT-CdSe nanocomposites possess a well-defined interface, thus significantly promoting the dispersion of CdSe within the P3HT matrix and facilitating the electronic interaction between these two components. The photophysical properties of nanocomposites were found to differ from the conventional composites in which P3HT and CdSe QDs were physically mixed. Solid-state emission spectra of nanocomposites suggested the charge transfer from P3HT to CdSe QDs, while the energy transfer from 3.5 nm CdSe QD to P3HT was implicated in the P3HT/CdSe composites. A faster decay in lifetime further confirmed the occurrence of charge transfer in P3HT-CdSe nanocomposites.

8:36AM A22.00004 Amplification of Self-Assembled Nanopatterns: Bilayer Approach to High Aspect-Ratio Cylindrical Nanopore Arrays and Their Use for Templating Functional Materials, HO-CHEOL KIM, IBM Almaden Research Center, OUN-HO PARK, JOY CHENG, MARK HART, ROBERT MILLER, HIROSHI ITO, IBM ALMADEN RESEARCH CENTER TEAM — Thin films containing well-defined nanoscopic cylindrical pores oriented perpendicular to the surface are highly desirable for a variety of applications. Of great interest is to use the porus structures for templating a variety of functional materials into 3D nanostructures. Previous reports employ the porous oxide of anodized aluminum or thin films of block copolymers for generating high aspect-ratio nanoporous films. It is, however, still desirable to develop a generalized, simple and reliable method to fabricate nanoporous templates with controlled pore dimensions, high aspect-ratio, substrate non-selectivity and uniformity over large areas. We report a relatively simple and reproducible method for generating nanoporous templates. The approach we used in this study provides nanoporous films with controlled pore diameters (8nm – 25nm in this study) and high aspect-ratio over large areas of a variety of substrates. We also report the application of the templates for generation of nanostructured copper sulfide and titania and their functional properties.

8:48AM A22.00005 Nanoparticle Arrays via Self Assembled Peptide Templates, NIKHIL SHARMA, MATTHEW LAMM, DARRIN POCHAN, University of Delaware — The bottom up approach towards nano-scale patterning presents the possibility of creating hierarchical architectures through simple self-assembly strategies. Herein, we demonstrate the use of a peptidic template for the construction of parallel, linear arrays of inorganic nanoparticles. A 20 amino acid peptide, consisting of alternating hydrophilic (lysine) and hydrophobic (valine) residues flanking a central diproline turn sequence (VKVKVKVVKVPPTKVKVKVKV-NH₂) was employed as a nano-scale template for the organization of 2nm gold particles. This peptide self assembles into a laminated fibrillar morphology in solution and has a periodic nanostructure consisting of alternating hydrophobic and hydrophilic layers with a lateral periodicity of 2.5 nm. Negatively charged gold nanoparticles are templated into the positively charged lysine layer through electrostatic interaction and are aligned within the template that itself swells to a periodic spacing of 4.0 nm in order to accommodate the particles. These 1D nanoparticle arrays have potential applications in fields like nano-electronics, and we are currently attempting to create arrays of quantum dots and hetero-structures of metal and semiconductor particles.

9:00AM A22.00006 Study of Alkanethiol Self-Assembled Structure Grown on Silver, LIANG HU, ZISHU ZHANG, MIKHAEL YU, EFREMOV, ERIC A. OLSON, MING ZHANG, LITO DE LA RAMA, LESLIE H. ALLEN, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Alkanethiol self-assembled structures grown on surface-supported Ag clusters (3D) are studied by measuring heat capacity with nanocalorimeter at high scanning rate (40,000 K/s), and compared with the self-assembled monolayer (SAMs) grown on planar Ag surface (2D). There is more amount of alkanethiol assembled on 3D Ag clusters compared with 2D SAMs, and the melting transition occurs at a higher temperature with sharper melting peak. This is due to the formation of layered Ag-alkanethiolate structure demonstrated by X-ray diffraction. IR spectrum indicates this self-assembled structure has a high degree of conformational order.

9:12AM A22.00007 Ordered Inorganic/Organic Composites via Novel Templates and Techniques, JAMES WATKINS, University of Massachusetts — The fabrication of well ordered nanocomposite materials offers new opportunities for device applications. Recently we reported that nanostructured templates with sub-10 nm domains can be easily obtained through the blending of disordered polymer surfactants containing poly(ethylene oxide) as the hydrophilic block with homopolymers including poly (acrylic acid), poly (4-vinyl phenol) and poly (stylene sulfonate) that selectively associate with the PEO block through hydrogen bonding. These inexpensive blends are strongly segregated, yielding well ordered domains. Moreover, the functionalities imparted by the homopolymers provide convenient handles for binding active materials such as nanoparticles and for promoting in situ, phase selective reactions to produce hierarchical metal oxide polymer composites. The behavior of the template systems and their use for the fabrication of well ordered polymer/nanoparticle, metal/oxide polymer, and metal oxide/polymer/nanoparticle composites using aqueous routes or via the 3-D replication of the template structure in supercritical fluids will be discussed.

9:48AM A22.00008 Two-Dimensional Confinement of Nanorods in Block Copolymer Domains, YU LIU, RANJAN DESHMIKH, RUSSELL COMPOSTO, University of Pennsylvania, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM — To control their unique electrical and optical properties, one-dimensional metallic-semiconductor nanoparticles need to be aligned and assembled within a host material. In our research, we investigated the assembly of gold nanorods (NRs) in films of a symmetric diblock copolymer, poly(styrene-b-methyl methacrylate), PS-b-PMMA (211kg/mol). The NR length and diameter was 42nm and 13nm, respectively. The NRs were grafted with a short PEG-brush (5kg/mol). During solvent annealing, the NRs become oriented as the PS-b-PMMA chains assemble into a parallel lamellar morphology. The NRs are selectively sequenced and confined in the PMMA domains, which are narrower than the NR length, due to the favorable interaction between the PEG brush and PMMA block. This confinement orients 71% of NRs within ± 5° of the lamella plane. This route to produce alternating layers containing conducting NRs separated by dielectric domains has the potential for fabricating self-assembled nanodevices. The thermal stability of the NRs in PS-b-PMMA and homo PMMA films will also be discussed.

10:00AM A22.00009 Surfactant Directed Assembly of ZnS Nanocrystals, YOU LI, CYRUS SAFINYA, JACOB ISRAELACHVILI, University of California Santa Barbara, NATALY BELMAN, YUVAL GOLAN, Ben Gurion University of the Negev, Israel — Post-synthesis assembly of nanocrystals into ordered two- and three-dimensional super-structures is an important step in many technological applications. A method was developed to use chain-crystalline surfactants to link nanocrystals into 2D and 3D assemblies with precise control of inter-particle distances as well as crystallographic orientation of the nanocrystals. X-ray diffraction and transmission electron microscopy data revealed that ZnS nanocrystals synthesized in octadecylamine (ODA) self-assemble into a highly ordered structure composed of stacked sheets with in-plane 2D-crystalline order. The unit cell of the nanocrystal superlattice (including type and dimensions) is directly related to the crystal structure of the pure surfactant, and thus can be tuned predictably by varying the surfactant chain length. This method can be used to assemble a broad range of nanocrystals and particles (Work supported by ONR N00014-05-1-0540, DOE DE-FG02-00ER46314, NSF DMR-0619171 and BSF 2002059).
10:12AM A22.00010 End-functionalized triblock copolymers as a robust template for assembly of nanoparticles1, RASTKO SKNEPNEK, JOSHUA ANDERSON, MONICA LAMM, JOERG SCHMALIAN, ALEX TRAVESSET, Iowa State University and Ames Lab — Polymers with attached end groups with specific affinity for nanoparticles, i.e., functionalized polymers, are shown to provide a robust templating strategy, where the aggregated nanoparticles follow the mesoscopic order imposed by the polymeric matrix. In this talk, we will present a detailed investigation of triblock polymer templating as a function of both nanoparticle size and concentration. Next to phases such as hexagons or gyroids, regularly observed in copolymer solutions and melts, we find a novel square columnar phase of two interpenetrating line-lattices of micellar cylinders and aligned nanoparticles. We argue that this phase is a realization of the packing problem of binary mixtures of disks. Our study suggests that nanoparticle templating with functionalized block copolymers can provide a simple and efficient tool for assembling novel materials with nanometer scale resolution.

1This research was supported by the U.S. Department of Energy-Basic Energy Science under contract no. DE-AC02-07CH11358.

10:24AM A22.00011 Nanoparticle Ordering in Diblock Copolymer-based Supramolecular Systems, THOMAS SCHILLING, UC Berkeley, MSE, TING XU, UC Berkeley, MSE & Chemistry, SHIH-HUANG TUNG, UC Berkeley, MSE, YUE WU, UC Berkeley, Chemistry — A well-controlled nanoparticle dispersion within a polymer matrix can have a significant impact on a wide range of material properties. A simple, efficient strategy to direct nanoparticle assembly within nanoscopic domains has been developed. Cadmium selenide (CdSe) nanoparticles were directly blended with diblock copolymer-based supramolecules wherein small molecules were attached to the side chain of one block via hydrogen-bonding. Co-assembly of nanoparticle and supramolecule were examined using SAXS and TEM, confirming fine orderning of the nanoparticles. The influence of nanoparticle concentration on supramolecule microphase separation and nanoparticle ordering was studied. Various functionalities should be readily incorportable into these systems by simply varying the nanoparticle type. The hierarchical assembly of supramolecule and nanoparticles presents many new opportunities for the fabrication of functional nanodevices.

10:36AM A22.00012 The metal insulator transition in self-assembled gold nanoparticle wires, M. E. REEVES, JIANWEI SUN, George Washington University, J. A. HOFFMANN, Applied Physics Laboratory, JASPER NIJDAM, George Washington University, QUEBRE TESSEMA, National Science Foundation, GWU/NP COLLABORATION — We report the temperature dependence of wires assembled from spherical nanoparticles by a relatively new technique, vertical colloidal deposition. This is a simple, one-step method for assembling spherical nanoparticles into wires without the need for lithographic templating. It is effective for a variety of conducting and nonconducting nanoparticles and substrates, and the only material requirement is that the nanoparticles be placed in a colloidal suspension that is wettable on the desired substrate. The shape of the meniscus defines the wire’s geometry, and we report the synthesis and physical properties of wires several millimeters long by a few micrometers wide. When wires are formed from 12 nm gold nanoparticles, they exhibit a weak metallic temperature dependence. Those assembled from 6 nm nanoparticles show activated behavior. Post-processing also affects the conductivity of the nanoparticle wires, such as when they are intercalated with proteins or other short organic molecules. Evidence for the metal insulator transition in these materials will be presented and discussed.

10:48AM A22.00013 Effects of Electric-Magnetic Fields on Hybrid Excitons in a Semiconductor Quantum Dot Coated by an Organic Shell, QUE HUONG NGUYEN, Marshall University, One John Marshall Drive, Huntington WV 25701 — The effect of electric and magnetic fields on the hybrid exciton of an organic-coated semiconductor spherical quantum dot is considered. Due to dipole-dipole interaction at the semiconductor dot-organic shell interface, a strong mixing of the Wannier-Mott exciton in the quantum dot and the Frenkel exciton of the organic medium occurs, resulting in a new hybrid exciton having priorities of both kinds of excitons as large exciton radius and large oscillator strength. The hybrid excitons are as sensitive to external perturbation as Wannier-Mott excitons. We investigate the effect of mutual presence of electric and magnetic fields on the hybrid exciton of the isolated semiconductor quantum dot such as CdSe (core) clothed by an organic or glass coating for two configuration of fields when the electric and magnetic fields are parallel and orthogonal. The fields affect the eigenfunctions (by a Stark -effect distortion and by the magnetic field-induced distortion) and the Frenkel-Wannier coupling term. Upon the application of the magnetic and electric fields the coupling term between the two kinds of excitons increases. The most important feature of this system is by adjusting the magnetic field and electric field, one can tune the resonance between the two kinds of excitons to get different regions of mixing to obtain the expected high non-linearity.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A23 DMP GMAG: Focus Session: Manganites

8:00AM A23.00001 Sliding charge density wave in manganites, SUSAN COX, NHMFL, Los Alamos National Laboratory — Stripe and checkerboard phases appear in many metal oxide compounds, and are thought to be linked to exotic behaviour such as high temperature superconductivity and colossal magnetoresistance. It is therefore extremely important to understand the fundamental nature of such phases. The so-called stripe phase of the manganites has long been interpreted as the localisation of charge at atomic sites. Here, we present resistance measurements on La0.50Ca0.50MnO3 which strongly suggest that this state is in fact a prototypical charge density wave (CDW) which undergoes collective transport. Dramatic resistance hysteresis effects and broadband noise properties are observed, both of which are typical of sliding CDW systems. Moreover, the high levels of disorder typical of manganites result in behaviour similar to that of well-known disordered CDW materials. The CDW-type behaviour of the manganite superstructure suggests that unusual transport and structural properties do not require exotic physics, but could emerge when a well-understood phase (the CDW) coexists with disorder.

8:36AM A23.00002 Polaron dynamics in La0.7Ba0.3MnO3 and La0.7Sr0.3MnO3, Y. CHEN, University of Maryland and NCNR, B. G. UELAND, J. W. LYNN, NCNR, S. BARILO, Institute of Solid State and Semiconductor Physics, Belarus, Y. MUKOVSKI, R. PRIVEZENTSEV, Moscow Institute of Steel and Alloys, Russia — In the perovskite manganites La1−xAxBi0.5MnO3 (A = Sr and Ba), the spin, lattice, charge and orbital degrees of freedom are intimately coupled, leading to a rich phase diagram. La0.7Ca0.3MnO3 (LCMO) is a metallic ferromagnet at temperatures below Tc ~ 257 K and colossal magnetoresistivity is observed and associated with the formation of nanoscale polarons that develop at elevated temperatures with an ordering wave vector of ~ (1/4,1/4,0). As the paramagnetic-insulating state is entered, a purely elastic component to the structural polaron scattering signals the development of the correlated polaron glass phase in LCMO. We investigated the structure and dynamics of these polarons through and above the ferromagnetic-paramagnetic-insulating transition by neutron scattering on single crystals of La0.7Ba0.3MnO3 and La0.7Sr0.3MnO3. In contrast to LCMO, no static polaron correlations are observed, however, we find that dynamic polaron correlations exist. We have measured the energy and temperature dependence of the dynamic polaron correlations. The formation of the dynamic polarons is not directly related to Tc.

This research was supported by the U.S. Department of Energy-Basic Energy Science under contract no. DE-AC02-07CH11358.
8:48AM A23.00003 Composition Dependence of Polaron Formation and Dynamics in La$_{1-x}$Ca$_x$MnO$_3$.

B.G. UELAND, Y. CHEN, J.W. LYNN, NIST Center for Neutron Research, Gaithersburg MD 20899, Y.M. MUKOVSKII, R. PRIVEZENTSEV, Moscow Institute of Steel and Alloys, Moscow 117936, Russia — The colossal magneto resistive perovskites La$_{1-x}$Ca$_x$MnO$_3$ have generated much interest due to the intimate correlation between their magnetic and transport properties. It is well known that for the doping range 0.22<x<0.47 a transition from a paramagnetic insulating to a ferromagnetic metallic state occurs upon cooling below T$_C$~150-250 K, and experiments have shown that the transition between these states is closely tied to the formation of lattice polarons. Recent neutron scattering experiments have directly observed that these polarons freeze into a glassy state at T=T$_M$, which is responsible for the first order phase transition at this level of doping. While it has been proposed that this glass state occurs at x=0, its dependence on doping and temperature has yet to be fully mapped out. Here we present results from elastic and inelastic neutron scattering experiments performed on single crystal samples of these materials for x=0.15, 0.2, and 0.25, which have been undertaken to determine the influence of the boundary for the glass phase evolves with x. Preliminary results indicate that in the insulating state (x<0.22), no static polaron scattering is observed (in zero field), in contrast to the results for the metallic regime.

9:00AM A23.00004 Current-induced persistent ferromagnetic metallic state in an Fe-doped manganite. HIDEAKI SAKAI, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo — A persistent ferromagnetic metallic state has been observed to be induced by excitation of an electric current for a single crystal of 7% Fe-doped (La$_{0.5}$Pr$_{0.3}$)$_x$Ca$_{0.2}$MnO$_y$, a typical "relaxor ferromagnet" [1] with coexisting clusters of the ferromagnetic metal and charge-orbital-ordered insulator. According to the simultaneous measurement of the resistance and magnetization, the induced ferromagnetic state is likely to form a filamentary pathway, where the increase in magnetization is estimated to be ∼0.4 μ$_B$/Mn. Distinguishing the current heating effect, which tends to conversely decrease the ferromagnetic fraction, from the intrinsic effect, we have successfully demonstrated the reproducible switching of both the resistance and magnetization by changing the magnitudes of the applied voltages.


9:12AM A23.00005 Terahertz time domain spectroscopy of ordered and disordered half-doped manganites. K.R. MAVANI, M. NAGAI, H. YADA, K. TANAKA, D.S. RANA, I. KAWAYAMA, M. TONOUCHI, DEPARTMENT OF PHYSICS, KYOTO UNIVERSITY, JAPAN TEAM, INSTITUTE OF LASER ENGINEERING, OSAKA UNIVERSITY, JAPAN COLLABORATION — Terahertz (THz) time domain spectroscopic studies were carried out on Nd$_{0.5}$Ca$_{0.5}$MnO$_3$ and Nd$_{0.5}$Ca$_{0.48}$Ba$_{0.02}$MnO$_3$ (NCBMO) charge-ordered (CO) manganite thin films. Temperature dependent complex optical conductivity (σ = σ$_1 + i$σ$_2$) was studied to probe the cation disorder effects on low energy charge dynamics. The frequency dependent σ$_1$ suggests formation of charge-density-waves in these manganites. A induced doping induced disorder, as in the case of NCBMO, weakens the CO state. However, at THz frequency, there are subtle effects of disorder on low frequency charge density wave critical temperature (T$_C$) and superexchange coupling is studied using Monte Carlo simulations. In the absence of on-site disorder, the model has a second order phase transition from a paramagnetic insulating phase to a ferromagnetic metallic phase in the CMR regime. The CMR effect is found to be associated with short-range charge and spin correlations in the insulating phase. This clearly shows that the CMR effect arises from the competition between the ferromagnetic (ferromagnetic) and insulating (paramagnetic) phases. In addition, our magnetic and transport data appear to imply that the paramagnetic-ferromagnetic (which gives rise to the CMR) occurs at a somewhat higher temperature, suggesting that it does not correspond to a threshhold of percolation between metallic and insulating states. The σ$_1$ and σ$_2$, both increase with temperature and show a scaling relationship, σ$_1$<σ$_2$, that is consistent with similar result observed for (PrCaSr)MnO$_3$ manganite. 2 Mavani et al., Europhys. Lett. (in print). 3 Pimenove et al., Phys. Rev. B 73, 220407(R).

This work is supported by JSPS through 'Grant-in-Aid for Creative Scientific Research' and 'Grant-in-Aid for Young Scientists (start-up)'.

9:24AM A23.00006 High Magnetic Field Time-resolved Optical Study of Manganites. PAULA SAHANGAMU, SANHITA GHOSH, STEPHÉN MCGILL, National High Magnetic Field Laboratory, Florida State University, HAIDONG ZHOU, BEN CONNER, CHRISTOPHER WIEBE, Department of Physics and NHMFL, Florida State University — We study the effects of applied electric fields and large magnetic fields on the optical properties of La$_{1-x}$Ca$_x$MnO$_3$ (x=0.18) (LCMO) and Pr$_{1-x}$Ca$_x$MnO$_3$ (x=0.5) (PCMO) using time-resolved techniques. Our measurements are performed from 4 K to room temperature and in magnetic fields up to 31 T. The conductivity of the low-temperature ferromagnetic state in LCMO is altered by the application of an electric field and these electrically-induced changes are further modified in the presence of an applied magnetic field. We demonstrate that time-resolved optical methods are capable of capturing these mixed electronic and magnetic effects. In addition, we performed time-resolved Kerr effect measurements in PCMO in an attempt to gain further insight into the loss of strong charge/orbital ordering in the presence of large applied magnetic fields.

This work is supported by the NHMFL through an IHRP grant.

9:36AM A23.00007 Properties of Doped Magnesio Oxide and the Origin of Colossal Magneto-resistance. I. FELNER, I. NOWIK, D. ORGAD, M. I. TSINDLEKHT, Hebrew Univ, Israel, A. FRYDMAN, D. I. GOLOSOV, N. OSSI, Bar-Ilan Univ, Israel, Y. M. MUKOVSKII, Moscow State Steel and Alloys Inst, Russia — We report a series of magnetic and transport measurements on high-quality single crystal manganate samples in the colossal magnetoresistive (CMR) regime. A small iron doping allows also for a Mössbauer spectroscopy study, showing both an unusual line broadening within the ferromagnetic phase and a coexistance of ferro- and paramagnetic contributions in the critical region. The resistance peak (which gives rise to the CMR) occurs at a somewhat higher resistivity than the CMR regime, suggesting that it does not correspond to a threshold of percolation between metallic (ferromagnetic) and insulating (paramagnetic) phases. In addition, our magnetic and transport data appear to imply that the paramagnetic-ferromagnetic (Curie) transition and the metal-insulator transition (the resistivity maximum) are two distinct phenomena on their own right, with distinct (although probably interrelated) physical origins. We speculate that these results can be understood phenomenologically within the framework of a two-fluid model.

9:48AM A23.00008 Monte Carlo study of the one-orbital model for manganites in the CMR regime. RONG YU, Department of Physics, University of Tennessee, CENGIZ SEN, GONZALO ALVAREZ, ORNL, ELBIO DAGOTTO, Department of Physics, University of Tennessee and Condensed Matter Sciences Division, ORNL — The thermal phase transition in the one-orbital model for manganites with cooperative phonons and superexchange coupling is studied using Monte Carlo simulations. In the absence of on-site disorder, the model has a second order phase transition from a paramagnetic insulating phase to a ferromagnetic metallic phase in the CMR regime. The CMR effect is found to be associated with short-range charge and spin correlations in the insulating phase. This clearly shows that the CMR effect arises from the competition between the ferromagnetic and a charge-ordered competing states. Motivated by a recent STM experiment, we also studied the local density of states in this one-orbital model. We show how the experimental results can be understood within our model.

10:00AM A23.00009 A New Correlated Model of Colossal Magneto resistive Manganese Oxides. D.I. GOLOSOV, Bar-Ilan University, Israel — A new minimal model is proposed for the doped manganese oxides which exhibit colossal magnetoresistance (CMR), involving (in addition to the ionics) a broad spin-majority conduction band as well as nearly localised-spin-minority electron states. We outline the reasons to introduce this model, and discuss some of its properties. In particular, a mean field analysis yields an interaction-induced enhancement of the interband hybridisation and implies an emergence of a small energy scale, linked to the longitudinal spin dynamics, charge fluctuations, and presumably also to the carrier transport. We suggest that these conclusions merit further theoretical and experimental investigation in the context of the CMR manganates.
10:12 AM A23.00010 Combined Effect of Bond- and Potential-Disorder in Half-Doped Manganites, SANJEEV KUMAR, University of Twente and Leiden University, ARNO KAMPF, University of Augsburg — We analyze the effects of both bond- and potential-disorder in the vicinity of a first-order metal insulator transition in a two-band model for manganites using a real-space Monte Carlo method. Our results reveal a novel charge-ordered state coexisting with spin-glass behavior. We provide the basis for understanding the phase diagrams of half-doped manganites, and contrast the effects of bond- and potential-disorder and the combination of both.

10:24 AM A23.00011 Nanoscale ferromagnetism and doping effect in manganites, S. M. YOSHIDOME, Osaka Prefecture University, Y. HORIBE, Rutgers University, T. ASA K, Y. MATSUI, NIMS, K. TAKENAKA, Nagoya University — We investigated temperature variation of ferromagnetic (FM) microstructures in La$_{1-x}$Sr$_x$MnO$_3$ ($x=0.175$) by low-temperature Lorentz microscopy. Also, changes of the FM domain structures by substituting non-magnetic Al$^{3+}$ ion for Mn one were examined. We succeeded in observing changes of magnetic domain structures from large FM domains with the average width of 1μm to stripe-shaped FM ones with the 100nm width in the metallic phase. On the other hand, the insulator phase was found in La$_{1-x}$Sr$_x$Mn$_{1-y}$Al$_y$O$_3$ ($x=0.175$, $y=0.02$). We found that the insulating phase exhibits a characteristic bi-modal distribution of the FM domains, which is characterized as the coexisting state of distinct types of the FM domains; one is the stripe-shaped FM domains and the other is the plate-shaped one. This mixture of distinct types of the FM domains breaks the coexistence of the conductivity and results in the insulating character in La$_{1-x}$Sr$_x$Mn$_1$-$x$$_y$Al$_y$O$_3$ ($x=0.175$, $y=0.04$).

10:36 AM A23.00012 Multiple Metal-Insulator Transitions in LPCMO Wires, T.Z. WARD, S.H. LIANG, K. FUCHIGAMI, University of Tennessee and Oak Ridge National Laboratory, L.F. YIN, Oak Ridge National Laboratory, E. DAGGOTTO, E.W. PLUMMER, J. SENH, University of Tennessee and Oak Ridge National Laboratory — The two hottest areas of research in condensed matter physics are complexity and nanoscale physics. Interestingly, these two areas have little overlap as most of the nanophysics research work is conducted using “simple” materials of metals or semiconductors instead of complex materials such as transition metal oxides (TMOs). However, due to the strong electronic correlation, it is exactly the transition metal oxides that will most likely lead to observations of new phenomena under spatial confinement. In this work, spatially confined La$_{325}$Pr$_{233}$Ca$_{375}$Mn$_3$O$_7$ (LPCMO) is shown to exhibit never before seen transport properties which reveal a double metal-insulator transition. These findings shine new light on the processes at play in LPCMO, as we use this novel technique to probe the material.

1Research sponsored by the U. S. Department of Energy under contract DE-AC05-000R22725 with the Oak Ridge National Laboratory, managed by UT-Battelle, LLC

10:48 AM A23.00013 Ferromagnetic tendencies at the surface of AF/CO bulk manganites, SHuai DONG, Rong YU, Seiji YUNOKI, Elbio DAGGOTTO, Department of Physics and Astronomy, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory — Previous investigations have shown that the surface of a ferromagnetic (FM) manganite has antiferromagnetic (AFM) tendencies. However, the development of ferromagnetism has been observed experimentally in some AFM charge-ordered (CO) manganites by reducing the grain size down to the nanoscale. Similar phenomena was also found in other nanosized CO oxides, such as La$_{1/3}$Sr$_{1/3}$FeO$_3$. To clarify these puzzling observations, using Monte Carlo techniques we studied the FM Kondo model, using open boundary conditions to simulate a surface. For some values of the couplings, the previously known tendency to an AFM outer shell was found for the case of a bulk FM state. But for other couplings, the opposite effect was observed: the existence of a FM layer at the surface of a AFM/CO material. Details will be provided in this presentation.

1Work supported by NSF DMR-0706020 and by the Division of Materials Science and Engineering, US DOE, under contract with UT-Battelle, LLC

Monday, March 10, 2008 8:00AM - 11:00AM — Session A24 DMP: Focus Session: Transport in Nanostructures I: STM and Atomic Control

8:00 AM A24.00001 Single electron tunneling measurements of Titanium Silicide islands on Si(100). J.L. TEDESCO, J.E. ROWE, North Carolina State University, R.J. NEMANICH, Arizona State University — Titanium silicide (TiSi$_2$) islands have been formed by the ultrahigh vacuum (UHV) deposition of thin films of titanium (< 1 nm) on clean Si(100) surfaces followed by annealing to ~800°C. Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been performed on these islands to demonstrate single electron tunneling (SET). Evidence of Coulomb staircase peaks corresponding to SET has been identified in current-voltage (I-V) curves recorded from islands at room temperature. Predictions of the orthodox model were found to agree with our data, except for slight discrepancies of the shape of the I-V curves at current steps. Many islands that were expected to exhibit SET did not do so. Potential reasons for the absence of SET include Schottky barrier lowering due to Fermi level pinning, and interfacial faceting which was identified as the most likely reason for the absence of observable SET. The positive SET results establish that a Schottky barrier can be used as an effective tunnel junction in a future double barrier tunnel junction (DBTJ) device. Possible approaches to improve the reliability based on control and engineering of surface and interface electronic bands will be discussed.

8:12 AM A24.00002 Tunneling Spectroscopy of Ultrathin Insulating Films: CuN on Cu(100), Charles D. RUGGIERO, TaeYoung Choi, Jay A. GUPTA, The Ohio State University — Insulating films comprising only a few atomic layers offer insight into the evolution of electronic structure at the nanoscale and are useful for controlling electronic coupling of adsorbates. We have studied the electronic structure of one monolayer thick CuN islands grown on Cu(100) with a low temperature (5K), ultrahigh vacuum scanning tunneling microscope. We find that CuN acts as an insulator, with a band gap that exceeds 4 eV. Measurements of the tunneling barrier height and image potential states indicate that the CuN work function is ~0.9 eV larger than bare Cu. This suggests a significant surface dipole, consistent with charge transfer predicted by theory. We find no significant dependence of these results on CuN coverage, from small islands (~ 10 nm$^2$) to complete films. This suggests that collective electronic structure is already established in the smallest islands. We use the CuN films to decouple metal nanoclusters from the Cu surface electron density. Tunneling spectra of few-atom Nb clusters on CuN reveal an atomic resonance that is not observed for clusters on Cu. http://www.physics.ohio-state.edu/~jagupta

1Supported by NSF CAREER (DMR-0645451)
8:24AM A24.00003 STM studies of transport through single azobenzene molecules1. TAELYOUNG CHOI, JAY A. GUPTA, Department of Physics, Ohio State University — A microscopic understanding of electrical contact to molecules is needed to improve the performance and reproducibility of devices based on organic materials. We use a low-temperature scanning tunneling microscope to study current flow through single molecules where the contacts and local environment are characterized with atomic resolution. Azobenzene was adsorbed on a Cu(100) surface partially covered with one-monolayer thick islands of CuN, an insulator with a bandgap exceeding 4 eV. Peaks in tunneling spectra attributed to molecular orbitals are observed for molecules on CuN, but not on Cu. This is consistent with the decrease in hybridization expected for adsorbates on insulating films. Current flow through azobenzene molecules which bridge Cu and CuN regions is highly asymmetric with bias voltage, suggestive of rectifying behavior. Atomically precise contacts can be made to the molecules by using the STM tip to manipulate nearby metal atoms. Spectroscopic imaging is used to monitor changes in molecular orbitals due to charge transfer to molecule and contacts.

1Supported by NSF CAREER (DMR-0645451)

8:36AM A24.00004 An atomic switch of electron propagation on Ge (001) by tunneling carrier injection. FUMIO KOMORI, Institute for Solid State Physics, The University of Tokyo — Reversible switching of electronic conduction through atom manipulation is one of the important subjects of nanoscience. However, different conducting pathways were not clearly observed with atomic resolution. We have demonstrated the correlation between the change of surface atomic position by tunneling carrier injection and that of the reflection of one-dimensional (1D) surface-state electrons on the Ge (001) surface with a low density of atomic Sn-Ge dimers.

[1] On the clean Ge(001) surface, two adjacent atoms form a buckled dimer, and the buckling orientation of the Ge dimer can be locally and reversibly controlled by carrier injection to the surface from the STM tip.

[2] The unoccupied surface π*-electron behaves like a 1D free electron along the Ge dimer row. When Sn atoms are deposited on the clean Ge(001) surface at room temperature, buckled dimers originating from the Sn atoms are formed at the Ge dimer position in the surface. [3] An atomic switch is realized for the π*-electrons in the Ge dimer row direction by injection carriers to reversibly flip the buckling orientation of a single Sn-Ge dimer in the dimer row. When the Sn atom of the heterogeneous dimer is at the lower position, the 1D electrons are reflected and a standing wave of this state is observed. Whereas, when it is at the upper position, the 1D electrons pass through the heterogeneous dimer, and no standing wave is observed. In this state, the lower atom of the dimer is Ge, and the π* state at the dimer is little different from that of the Ge-Ge dimers.


9:12AM A24.00005 Quantum Channels and Conductance Oscillations in TiOx Nano-switches. FENG MIAO, Department of Physics and Astronomy, University of California, Riverside; J. JOSHUA YANG, DUNCAN R. STEWART, R. STANLEY WILLIAMS, HP labs, Palo Alto, CHUN NING LAU, Department of Physics and Astronomy, University of California, Riverside — We investigate conductance switching in Pt/TiOx/Pt devices by pressure-modulated conductance microscopy. For devices with conductance G > GQ, and G < GQ, where GQ is the conductance quantum, localized pressure-induced conductance peaks are observed, indicating formation of nanoscale conductance pathways on the electrodes. We postulate that these nano-conducting channels are related to the drift of oxygen vacancies under electrical field. For devices with G > 1-2 GQ, in addition of conductance peaks, we also observed conductance dips and oscillations in response to localized pressure. These results suggest formation of quantum conductance channels in our devices, and can be modeled by considering interfering electron waves between two partially transmitting electrodes. Our findings suggest the possible use of these devices as atomic-scale switches.

9:24AM A24.00006 Electronic switching in nanoscale titanium oxide devices, DUNCAN STEWART, Hewlett-Packard Laboratories, Palo Alto, CA USA, J. JOSHUA YANG, JULIEN BORGHETTI, DOUGLAS OHLBERG, MATTHEW PICKETT, FENG MIAO, R. STANLEY WILLIAMS — Titanium metal is widely used as a top metal contact for nanoscale molecular electronic devices, where it has been assumed to form a few-atom-thick Ti carbide overlayer. Using a vacuum delamination technique we expose and analyze chemically pristine buried titanium/organic monolayer interfaces from devices that have displayed ‘molecular electronic switching’. We establish that under many conditions the titanium instead forms a few-nanometer-thick Ti carbide overlayer. Using a vacuum delamination technique we expose and analyze chemically pristine buried titanium/organic monolayer interfaces from devices that have displayed ‘molecular electronic switching’. We establish that under many conditions the titanium instead forms a few-nanometer-thick Ti carbide overlayer.

9:36AM A24.00007 Electron transport simulations through organic adlayers on metal surfaces1, MANUEL COBIAN, ICMAB - CSIC, NICOLAS LORENTE, PABLO ORDEJON, CIN2 - CSIC — Molecular entities at the interface with an inorganic surface are the basis for new hybrid functional materials for microelectronics. In most cases, strong bonding of molecules to metal surfaces perturbs the discrete molecular energy levels leading to a broadening of the molecular density of states. Deposition of C60 on a Au(111) surface previously exposed to tetraphenyladamantane give rises to a nanostructured organic layer where the electronic coupling between the C60 and the Au(111) surface is significantly reduced compared to C60 on a clean Au(111) surface. Calculations based on Density Functional Theory reveal that intermolecular interactions lock C60 into a particular orientation in agreement with Scanning Tunneling Microscopy experiments. This system exhibits the presence of negative differential resistance which can be understood by simulations of the transport properties at the ab-initio level using TRANSIESTA.

1supported by Spanish MEC (No FIS2006-12117-C04-01)

9:48AM A24.00008 Scanning tunneling spectroscopy (STS) of DNA and G4-DNA molecules1, DANNY PORATH, Physical Chemistry Department and Center for Nanoscience and Nanotechnology, The Hebrew University, Jerusalem 91904, Israel, ERREZ SHAPIR, HEZY COHEN, Hebrew University, Israel, ALEXANDER KOTLYAR, Tel Aviv University, Israel, ROSA DI FELICE, INFM-CNR, Modena, Italy — Attempts to resolve the energy level structure of single DNA molecules by STS span over the last two decades, thanks to this technique ability to probe the local density of states of objects deposited on a surface. Success was hindered by extreme technical difficulties in stable deposition and reproducibility. By using STS at 78 °K, for the first time we disclose the energy spectrum of poly(G)-poly(C) DNA molecules deposited on gold. The tunneling current-voltage characteristics and their derivative curves exhibit a clear gap and a peak structure around the gap. By means of ab initio Density Functional Theory calculations the character of the observed peaks is consistent to orbitals originating from the different molecular components. Limited fluctuations in the I-V curves are observed and statistically characterized.

1Funding was provided by the EC through contracts IST-2001-38951 (“DNA-Based Nanowires”) and FP6-029192 (“DNA-Based Nanodevices”).
10:00AM A24.00009 Microscopic Characterization of Organic/Metal Interfaces: a Combined DFT and Many-Body Perturbation Theory Study , YAN LI, DEYU LU, GIULIA GALLI, University of California, Davis — Aromatic molecules and molecular assemblies have received widespread attention as possible components of molecular electronic devices. An essential prerequisite to understand their stability and transport properties is the microscopic characterization of the interface formed with metallic leads. We present a comprehensive, first-principles study of the interface of Au(111) and a representative aromatic isocyanide molecular SAM (phenylenediisocyanide). We provide predictions about the binding geometries, coverage and stability properties, which are in good agreement with experimental measurements. We also discuss the electronic properties of the organic/metal interface by including self-energy corrections through many-body perturbation theory (GWA), and surface polarization effects. Our results indicate that electronic structure calculations beyond DFT are required to make an accurate assessment of energy level alignments between SAMs and the metallic leads.

10:12AM A24.00010 Scanning tunneling spectroscopy of mass selected Ag clusters on C_{60} functionalized surfaces1 , HEINZ HÖVEL, STEFANIE DUFFE, LUKAS PATRYARCHA, Technische Universität Dortmund, Experimentelle Physik I, Germany, CHUNRONG YIN, BERND VON ISSENDORFF, Universität Freiburg, Fakultät fuer Physik, Germany, MICHAEL MOSELER, Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg, Germany — Scanning tunneling spectroscopy (STS), which can be used to study the electronic properties of individual clusters on surfaces [1] is combined with the deposition of mass selected Ag clusters (from Ag_{95}^{+} to Ag_{56}^{+}). A functionalization of the substrate with C_{60} layers proved to be very useful to ensure the soft landing of the clusters and to bind them to fixed positions on the surface [2]. The knowledge of the exact cluster size shows that one has to interpret the STS derived cluster height carefully, considering details of the STM imaging process. For the soft landed clusters we measured identical spectral features for individual clusters with the same selected size using STS at 5 K.

1Work supported by the Deutsche Forschungsgemeinschaft (SPP 1153)

10:24AM A24.00011 Rectification in Porphyrin/Fullerene Dyads on Au(111)*, DOMINIC BRITTI, RAY PHANEUF, University of Maryland, FRANCESCA MATINO, VALENTINA ARIMA, MANUEL PIAZENZA, FABIO DELLA SALA, GIUSEPPE MARUCCIO, NNL Lecce, Italy, ROBERTA DEL SOLE1, GIUSEPPE MELE, GIUSEPPE VASAPOLLO, Universita del Salento, Italy, ROBERTO CINGOLANI, ROSS RINALDI, NNL Lecce, Italy — We present an ultrahigh vacuum scanning tunneling microscopy (UHV-STM) and scanning tunneling spectroscopy study of ex-situ self assembled supramolecular dyads, consisting of fulleropyrrolidines (PyC_{2}C_{60}) axially ligated to zinc(II) tetraphenylporphyrin (ZnTPP), self organized by axial ligation to a 4-aminophenol (4-ATP), self assembled monolayer on gold (111). By highly diluting the PyC_{2}C_{60} solution, and subsequently annealing in vacuum, isolated dyads are obtained; these show both bias polarity-dependent apparent height in STM images, and highly rectifying behaviour in tunneling spectroscopy. First principles density functional theory calculations clarify the conformational and the electronic properties of the 4-ATP/ZnTPP/PyC_{2}C_{60} system. The rectifying behavior is explained using a model based on the Aviram-Ratner mechanism. * Work supported by the CNR-INFM, by a NSF US-Italy Cooperative Research Program #OISE-0242579, by the SpiDME European project and by MIUR FIRB 2003 ‘SYNERGY’ grant. Lab for Physical Sciences and in part by a NSF-MRSEC, DMR# 0520471.

1Università del Salento, Italy

10:36AM A24.00012 Electron transport study of surface-supported nanostructures with a quadruprobe scanning tunneling microscope1 , TAE-HWAN KIM, JOHN WENDELKEN, AN-PING LI, Oak Ridge National Laboratory — We report the study of the electron transport and structural properties of nanostructured materials with a low temperature quadruprobe scanning tunneling microscope (STM) system. Self-assembled nanostructures including epitaxially grown nanowires and atomic chains have been fabricated by doping with small amounts of metal atoms (Au, Gd, Y, Ag) on a Si surface. The local electronic states and transport properties have been characterized in situ. This research took the advantage of our recent development of the quadruprobe STM system. As a "nano" version of a four-probe station, the quadruprobe STM system provides an integrated research platform with a low temperature four-probe STM, a molecular-beam epitaxy growth chamber, a high resolution scanning tunneling microscope, and a scanning Auger microscope. The four STM probes can be driven independently with sub-nanometer precision, enabling conventional STM imaging and four-point electrical transport study of surface electronic systems and nanostructured materials at temperatures down to 10 K.

1This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.

surface of the film. The surface tension obtained from static grazing incidence scattering data shows that a PDMS layer segregates to the free angle, the surface dynamics and the micelle dynamics were selectively measured. The obtained viscosity will be compared with the value from the mechanical copolymers films used in this study have an internal structure of spherical micelles. This ought to have a strong influence on the physical properties of the
ZHANG JIANG, SUNIL K. SINHA, Dept. of Physics, University of California San Diego, A. RUEHM, Max Planck Institute for Metals Research, Stuttgart, HEEJU LEE, YOUNG JOO LEE, SANGHOON SONG, Dept. of Physics & Interdisciplinary Program of Intergrated Biotechnology, Sogang University, Korea, consider an ideal two-dimensional system, the creation of various structures using laser lithography provides an excellent probe for studying instabilities in two instability, which results in the breaking up of an extended cylinder into an arrangement of smaller, evenly spaced droplets. Since our diblock system can be films allows us to produce structures far smaller than those imposed by the resolution of the laser patterning procedure. An example of this is the Plateau-Rayleigh Brockhouse Institute for Materials Research, McMaster University — We have developed a novel surface tension-driven laser lithography technique that enables 8:00AM A25.00001 Control of P(S-b-PMMA) Orientation on Organosilicate Substrates by Thermal Treatment, KOOKHEON CHAR, HYOSEON SUH, Seoul National University — One of most important factors to control the orientation of microdomains in block copolymer films is the wetting behavior of a block copolymer at an interface. From this perspective, we studied the wetting behavior of P(S-b- MMA) block copolymer (BCP) thin films on silesquioxane-based organosilicate (OS) substrates, which have potential applications as interlayer dielectrics (ILDs) for next generation semiconductor devices. We controlled the surface energy of OS substrates by changing the treatment temperature. As the treatment temperature was increased, the wetting behavior of a P(S-b-MMA) film on OS substrates changed from the asymmetric to the symmetric wetting, which allowed us to find the optimum treatment temperature for the neutral wetting behavior. Changes in the orientation of BCP microdomains on OS substrates were analyzed by AFM, FE-SEM, and GI-SAXS. These results show the potential that the OS ILDs prepared in this study do not require any additional surface modifications such as random copolymer brushes or SAMs for BCP microdomains to orient perpendicular to the substrate, which could ultimately be applied to BCP lithography.

8:12AM A25.00002 Functionalization of PEO Nanocylinder Array Structure in Block Copolymer Thin Film, KAORI KAMATA, JST-PRESTO, TOMOKAZU IYODA, Tokyo Institute of Technology — Phase-separated nanostructure of block copolymer has been intensively studied as one of the most promising candidates for many important nanotechnological applications, because the feature size of domain structure generated by block copolymers is ranging to a level of several nanometers. We have studied the nanostructures of block copolymers, which are based on the use of amphiphilic block copolymer, PEO-b-PMA(Az), to establish the long range orderness onto the substrate. Here, we describe the nanotemplating process with domain selective doping of PEO cylindrical domains, using various kinds of metal cation sources, such as Fe or Pb ions. Furthermore, the ionic liquid also hybridized into the PEO nanocylinders to form liquid nanochannels perpendicular to the substrate. A wide variety of cations were successfully incorporated through the coordination bonding with the oxygen in PEO chain. The resulting metal cation hybrid films could offer the metallic nanopillar arrays, with the nanostructure-specific electrochemical, electric or magnetic properties.

8:24AM A25.00003 Block copolymer mask with cylindrical nanochannels for wet nanopatterning on silicon wafer, RYOKO WATANABE, KAORI KAMATA, TOMOKAZU IYODA, Division of Integrated Molecular Engineering, Chem. Res. Lab., Tokyo Institute of Technology — Microphase-separated structure of block copolymer (BC) thin films has been considered as a mass-productive nanomask, in which the periodicity of the pattern can be tuned by molecular weight. We have developed a series of amphiphilic BC, PEO<sub>n</sub>-b-PMA(Az)<sub>m</sub>, consisting of hydrophilic, ion-conductive poly(ethylene oxide) (PEO) and hydrophobic poly(methacrylate) with azobenzene in its side chain. This BC forms hexagonally arranged PEO cylinders which span across the thickness of the film after thermal annealing. In this study, PEO cylinders were blended with poly(ethylene glycol) monomethylether to provide effective nanochannel that can perpendicularly diffuse etching species for wet etching of silicon wafer. As a quick and total wet nanopatterning process, a silicon wafer covered by the BC mask was annealed at 140 degrees C for 1 h and immersed into 33 wt.% NH<sub>4</sub>F aqueous solution for 3 min. AFM observation of the resulting silicon wafer surface revealed a hexagonally arranged nanohole array with 24 nm of center-to-center distance and 10 nm of diameter was fabricated.

8:36AM A25.00004 Is a short fluorinated segment sufficient to induce interfacial rearrangements in diblock co-polymers?, UMESH SHRESTHA, DVORA PERAHIA, Clemson University, STEPHAN CLARSON, University of Cincinnati — The interfacial structure of thin diblock co-polymer films is a result of internal segregation between the blocks and their affinity to the interfaces. Introducing a fluorinated group affects significantly the segregation of the fluorinated block to the interface. The interfacial structure and dynamics of thin layers of a diblock co-polymer Polytetrafluoro propyl methyl siloxane-polystyrene (PTEPMS-PS) with the fraction of the fluorinated block ranging from 0.03 to 0.5 was studied by neutron reflectivity. The uniqueness of this diblock lies in the presence siloxane group and a fluorinated group intercalated into one of the where the siloxane offers flexibility and the fluorine exhibits low interfacial energies. While the air interface is dominated by fluorinated segments for all volume fractions, layering is observed even for the shortest fluorinated segments. The rate of rearrangement upon annealing varies with the size of the fluorinated block.

8:48AM A25.00005 Multi-block copolymers in thin films, PANAGIOTIS MANIADIS, EDWARD KOBER, TURAB LOOKMAN, Los Alamos National Laboratory, Los Alamos NM — We study the behavior of an {AB}, multi-block copolymer confined to a thin film, using self consistent field theory (SCFT) methods. Due to the breaking of symmetry in the direction of confinement, the propagators do not obey the usual diffusion equation. We derive the diffusion equation which correctly describes the confined polymer system and find that it differs from the original in an area which is approximately 3 times the Kuhn length of the polymer, close to the surface of the film. We use the modified diffusion equation to study the structure of the confined polymer.

9:00AM A25.00006 Two-Dimensional Instabilities in Patterned Diblock Copolymer Films, JOSEPH PARETE, Department of Engineering Physics and the Brockhouse Institute for Materials Research, McMaster University, ANDREW B. CROLL, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, JOHN S. PRESTON, Department of Engineering Physics and the Brockhouse Institute for Materials Research, McMaster University, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — We have developed a novel surface tension-driven laser lithography technique that enables the effective generation of microstructures in polymer systems. Combining this approach with naturally occurring instabilities in symmetric diblock copolymer films allows us to produce structures far smaller than those imposed by the resolution of the laser patterning procedure. An example of this is the Plateau-Rayleigh instability, which results in the breaking up of an extended cylinder into an arrangement of smaller, evenly spaced droplets. Since our diblock system can be considered an ideal two-dimensional system, the creation of various structures using laser lithography provides an excellent probe for studying instabilities in two dimensions. Optical and atomic force microscope measurements are presented and discussed in terms of a linear stability analysis.

9:12AM A25.00007 Structure and dynamics of block copolymer films by XPCS, HYUNJUNG KIM, HEEJU LEE, YOUNG JOO LEE, SANGHOON SONG, Dept. of Physics & Interdisciplinary Program of Intergrated Biotechnology, Sogang University, Korea, ZHANG JIANG, SUNIL K. SINHA, Dept. of Physics, University of California San Diego, A. RUEHM, Max Planck Institute for Metals Research, Stuttgart, Germany — We have measured the structure and the dynamics of block copolymer films in the melt using X-ray Photon Correlation Spectroscopy. Block-copolymers films used in this study have an internal structure of spherical micelles. This ought to have a strong influence on the physical properties of the thin films. The results from the surface dynamics are compared with the theory of overdamped thermal capillary waves on thin films. By changing the incident angle, the surface dynamics and the micelle dynamics were selectively measured. The obtained viscosity will be compared with the value from the mechanical measurement of the bulk material. The surface tension obtained from static grazing incidence scattering data shows that a PDMS layer segregates to the free surface of the film.

<sup>3</sup>Work supported by Korea Science and Engineering Foundation (R01-2007-000-11808-0) and Seoul Research and Business Development Program (10816)
9:24AM A25.00008 Sphere-Forming and Cylinder-Forming Block Copolymer Thin Films Aligned Under Double Shear. ANDREW MARENIC, RICHARD REGISTER, Princeton University, PAUL CHAIKIN, New York University — Studies have shown that stress transmitted through a viscous layer to a sphere- or cylinder-forming block copolymer thin film can orient the microdomains in the direction of the imposed shear. For the creation of complex patterns, reorientation of these unidirectionally oriented films is necessary. Here we demonstrate the ability of shear to realign the microdomains along a second direction, as imaged by atomic-force microscopy. The results are in qualitative agreement with our previously proposed phenomenological model; however, the stress required for realignment is larger (factor of 2.7 for sphere-formers and factor of 1.2 for cylinder-formers) than the stress required to orient a film from the polycrystalline state. We also observed grain boundary generation within the transition region between alignment with the first shear direction and alignment with the second shear direction. No noticeable change in the dislocation density or its angular distribution was observed in the sphere-forming block copolymer thin films following the second shear.

9:36AM A25.00009 Rapid Directed Assembly of Block Copolymer Films on chemically patterned surfaces at Elevated Temperatures. ADAM WELANDER, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin, Madison — We report on the rapid directed assembly of poly(styrene-b-methyl methacrylate) (PS-b-PMMA) block copolymer thin films at elevated temperatures well above the glass transition temperature ($T_g$) on chemically patterned surfaces. The time needed for defect free assembly, where the chemical pattern ($L_S$) closely matches the natural length of the block copolymer ($L_0$), is strongly dependent on the annealing temperature. Annealing times range from 150 minutes at 180 °C to 3 minutes at 230 °C. This system behavior is well described as a simple thermally activated process with an apparent activation energy ($\Delta E_a$) of 182 kJ/mol and a polymer diffusion coefficient of 7.5E-15 cm²/s⁻¹ at 190 °C. Modeling this behavior predicts annealing times of 13.5 seconds at 250 °C and 1.9 seconds at 280 °C. While these times are difficult to investigate experimentally, a one minute anneal at these elevated temperatures not only shows perfect assembly where $L_S = L_0$, but also where $L_S < L_0$.

9:48AM A25.00010 Precise Control of 3-dimensional Block Copolymer Assembly using 2-dimensional Chemical Templates. SANGCHEOL KIM, Polymers Division, NIST/Dept. of Materials Science and Engineering, University of Maryland, HAE-JEONG LEE, RONALD L. JONES, ALAMGIR KARIM, Polymers Division, NIST, R.M. BRIBER, Dept. of Materials Science and Engineering, University of Maryland, HQ-CHEML KIM, Almaden Research Center, IBM — Chemically heterogeneous substrates, where the periodicities of the chemical pattern are close to those of lamellae microdomains of block copolymers, have been used as an effective route to align the microdomains with a low number density of defects. Macroscopic chemical heterogeneity is, however, still valuable for providing insights on ordering behavior of block copolymers. Using a series of chemical patterns with micrometers length scales, we studied the wetting and self-assembly behavior of poly(styrene-b-methyl methacrylate) (PS-b-PMMA). We found that the variation in morphology and orientation of microdomains are governed by the degree of chemical contrast and the size of the underlying chemical patterns. The two-dimensional chemical template is shown to precisely control the three dimensional assembly of the block copolymer film.

10:00AM A25.00011 Novel Complex Nanostructures from Directed Assembly of Block Copolymers on Incommensurate Surface Patterns. SANG OK KIM, BONG HOON KIM, Materials Science and Engineering, KAIST, South Korea, HARUN H. SOLAK, Paul Scherrer Institute, Switzerland, DONG MENG, QIANG WANG, Chemical and Biological Engineering, Colorado State University, USA — Self-assembled nanostructures of block copolymer thin films have attracted enormous attention as useful templates for nanofabrication. We present that a chemically nanopatterned surface prepared by photolithography is able to direct the assembly of a block copolymer thin film to form a novel complex nanostructure. When a cylindrical block copolymer was assembled on a stripe pattern, whose pattern period was twice as large as a natural lattice size of the bulk nanostructure, a new structure was produced, where cylinders were alternately oriented parallel and perpendicular to the surface. Self-consistent field calculations supported the emergence of the new structure, providing insight into the detailed structure and formation mechanism. Our work suggests that the combining top-down and bottom-up approaches may provide a versatile pathway for fabricating well-registered complex nanostructures, potentially useful in diverse advanced applications. References; S. O. Kim, et al. Nature 424, 411 (2003); M. P. Stoykovich, et al. Science 308, 1442 (2005); S. O. Kim, et al. Macromolecules 39, 5466 (2006); S. O. Kim, et al. Advanced Materials 19, 3271 (2007).

10:12AM A25.00012 Templated Self-Assembly of Asymmetric Ternary Blends of Block Copolymers and Homopolymers1. KARL STUEN, FRANCOIS DETCHEVERRY, CARLA THOMAS, Univ. of Wisc. - Madison Dept. of Chem. and Biol. Eng., RICHARD FARRELL, CRANN, Dept. Chem. Univ. Coll. Cork, Tyndall Nat. Inst., IRELAND, MICHAEL MORRIS, CRANN, Dept. Chem. Univ. Coll. Cork, Ireland, JUAN DE PAULO, PAUL NEALEY, Univ. of Wisc. Madison Dept. of Chem. and Biol. Eng. — Template assembly of ternary blends of cylinder-forming PS-block-PMMA and homopolymers of PS and PMMA was investigated experimentally and with Monte Carlo simulations of a coarse-grained model. The blends were deposited into trench features coated with a neutral brush to induce cylinder orientation perpendicular to the substrate. The ternary blends were used to systematically control the commensurability between the blend and trenches of constant width. Important patterning parameters such as the degree of perfection, the domain spacing perpendicular and parallel to the confining template, the domain uniformity, and shape of the unit cell were quantified as a function of blend composition. The cylindrical nanostructures appear to have improved uniformity across the trench width compared with spherical systems.

1Supported by the Semiconductor Research Corporation, the NSF NSEC at UW-Madison, CRANN, and SFI CSET Prog. Ireland. Materials and support provided by Intel.

10:24AM A25.00013 Directed Assembly of Asymmetric Ternary Block Copolymer-Homopolymer Blends Thin Films on Checkerboard Trimming Chemical Pattern. HUIMAN KANG, PAUL F. NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin, Madison, WI 53706 USA — Typical 2-dimensional projections of ordered block copolymer morphologies in thin films include periodic lines or hexagonal arrays of spots and therefore may not be suitable for patterning even strictly periodic device-oriented arrays, such as checkerboard trimming patterns (alternating lines and dashed lines) used in the fabrication of dynamic random access memory (DRAM). Here we direct the assembly of asymmetric ternary polystyrene-block-poly(methylmethacrylate) (PS-b-PMMA)/homopolymer PS/homopolymer PMMA blends on checkerboard trimming chemical patterns. The degree of perfection and domain uniformity of the assembled films was quantified as a function of overall composition of PS or PMMA and total homopolymer fraction in the blends. By matching polymer volume fractions and pattern area fractions, blends composed of lamellae-forming block copolymer and substantially asymmetric fractions of the two homopolymers could be assembled into equilibrated line and dash morphologies.
10:36AM A25.00014 Influence of added copolymers on thin film polymer blends studied by atomic force microscopy: surface morphology and dewetting. DEAN WALDOW, JENIFER HOFFERT, KRIS PETERSON, Pacific Lutheran University — Atomic force microscopy (AFM) was used to study thin film polymer blends of polystyrene (PS) and polybutadiene (PB). These blends were studied with increasing concentration of block, random, and graft copolymers. Thin films were prepared by spin coating from a good solvent, which resulted in film thicknesses of approximately 65 nm. The AFM data were collected in AC mode and included both topographic and phase data. The topography data were analyzed using lateral Fourier Transform analysis as well as real space techniques both lateral and normal to the surface. The results suggest that lateral phase separated domain size decreases with increasing copolymer concentration for each of additives studied and for all concentrations.

10:48AM A25.00015 Controlled Dimensions of Nanostructures in Asymmetric Ternary Blends of Block Copolymers and Homopolymers in Thin Films. CARLA THOMAS, KARL STUEN, - Madison Dept. of Chem. and Biol. Eng., NICOLÁF FERRIER, Univ. of Wisc. - Madison Dept. of Mech. Eng., PAUL NEALEY, Univ. of Wisc. - Madison Dept. of Chem. and Biol. Eng. — Ternary blends of cylinder-forming PS-block-PMMA and homopolymers of PS and PMMA were investigated in thin films on a neutral brush with the domains oriented perpendicular to the substrate. Five blends with homopolymers having different degrees of polymerization (N) were studied to quantify the dimensional scaling of the domains and suitability for patterning. In the dry brush regime, the best pattern uniformity and fewest defects were found when N of the homopolymers matched N of the corresponding block of the block copolymer. The lattice spacing of the cylindrical array, D, and cylinder diameter uniformity changed with φPS, the homopolymer volume fraction in the film, and N of the homopolymers. With the ternary blends, D could be increased up to 200 percent relative to the neat block copolymer; the ternary blends allow φPS greater than 0.4 without inducing a phase change.

1Supported by the Semiconductor Research Corporation and the NSF NSEC at UW-Madison.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A26 DCP: Focus Session: Photophysics of Cold Molecules I Morial Convention Center 218

8:00AM A26.00001 Isolation of Molecules in Helium Nanodroplets: Spectroscopy and Dynamics at Ultra-cold Temperatures , FRANK STIENKEMEIER, University of Freiburg — The isolation of atoms, molecules, clusters or nano-sized complexes in helium nanodroplets allows detailed spectroscopic studies at temperatures in the millikelvin range. Moreover, femtosecond real-time spectroscopy has been introduced to study dynamical processes in the ultracold helium environment. On the one hand, wave packet propagation opens a window to dynamical processes, allowing even a view to superfluid properties at the nanoscale. This is exemplified at decoherence effects in the wave packet propagation of small molecules attached to the droplets. On the other hand, high-resolution mass spectra using both femtosecond photoionisation (PI) as well as electron impact ionization enable us to characterize reactive processes at temperatures in the millikelvin range. As an example, alkali cluster – water complexes are formed in helium droplets. By recording multi-photon PI spectra we can distinguish between reactive processes of the neutral clusters and ionic reactions occurring after ionisation of the alkali cluster component. These studies pave the way to time-resolved reaction dynamics at very low temperatures.

8:36AM A26.00002 Nonequilibrium magnesium complexes formed in helium nanodroplets. JOSEF TIGGESBAUMKER, ANDREAS PRZYSTAWIK, SEBASTIAN GODE, KARL-HEINZ MEIWES-BROER, Institute of Physics, University of Rostock, 18051 Rostock, Germany — Doping helium droplets with alkaline earth atoms is an interesting tool to investigate the interaction with the superfluid helium. Magnesium is a corner case regarding the degree of solvation in helium [1,2] which may enable the detection of quantized vortices in helium droplets. In this contribution we add another facet to the discussion. The absorption of helium droplets doped with magnesium atoms is measured with resonant two-photon ionization at different concentrations of droplet size and the number of doped Mg atoms. This enables the unambiguous identification of the absorption of an isolated atom inside the droplet centered around 279 nm. When increasing the Mg content of the droplet we find evidence for the formation of metastable, weakly bound Mg complexes. After excitation of such a complex it collapses to a Mg cluster on a timescale of 20 ps.


8:48AM A26.00003 Superfluid ⁴He density functional theory in 2-D cylindrical coordinates. JUSSI ELORANTA, SEAN FRENCH, Department of Chemistry and Biochemistry, California State University at Northridge, STEVEN FIEDLER, Department of Chemical Engineering, The University of Michigan — Bosonic density functional theory describing superfluid ⁴He is formulated in 2-D cylindrical coordinates and a numerical implementation of the model using a regular spatial grid basis is presented. The 2-D formulation has many important applications as the 1-D treatment cannot, for example, describe translational motion of atoms and molecules solvated in the liquid and the 3-D theory is usually computationally too expensive, especially when describing dynamics in bulk superfluid ⁴He. The theory is implemented in both real and imaginary time forms for allowing solution of both time-dependent and time-independent problems. Two test cases for the developed method are presented and the results are compared against the previously published results. Finally, the method is applied to describe solvation of single wall carbon nanotubes in superfluid ⁴He at 0 K and the implications of the results to dynamic liquid response are discussed.

1Support from Research Corporation is acknowledged.

9:00AM A26.00004 Photo-induced isomerization and chemical reaction dynamics in superfluid helium droplets. JEREMY MERRITT, GARY DOUBERLY, ROGER MILLER, University of North Carolina-Chapel Hill — Near threshold photo-induced isomerization and photo-induced chemical reactions have long been sought after as sensitive probes of the underlying potential energy surface. One of the most important questions asked is how the initially bright quantum state couples to the reaction coordinate, and thus relates to energy transfer in general. Helium droplets have now allowed us to stabilize entrance channel clusters behind very small reaction barriers such that vibrational excitation may result in reaction. Through two examples, namely the isomerization of the 2 binary complexes of HF-HCN {Douberty et al. PCCP 2005, 7, 4633}, and the induced reaction of the gallium-HCN complex {Merritt et al. JPCA 2007, DOI:10.1021/jp074981e} we will show how the branching ratios for reaction and predissociation can be determined and the influence of the superfluid He solvent.
9:12AM A26.00005 Rydberg States of Na-doped Helium Nanodroplets, MARCEL DRABBELS — The dynamics of excited states of Na atoms deposited on the surface of helium nanodroplets has been investigated with velocity map ion imaging, photoelectron spectroscopy and time-of-flight mass-spectroscopy. For the first time, the excitation spectra of Na-doped helium nanodroplets corresponding to Rydberg states of Na atoms have been measured from the lowest excited 3p state up to the ionization threshold. All lines in the excitation spectra are shifted and broadened with respect to the corresponding atomic lines. In addition to bare Na* atoms also NaNaHe (N = 1-6) exciplexes are detected upon excitation. Photoelectron spectroscopy reveals the desorption of Na* not only in the initially excited states but also in lower lying states, indicating that relaxation plays an important role. The recorded velocity distributions show interesting characteristics: for the lowest states the mean kinetic energy of Na* increases linearly with excitation energy. The velocity distributions of NaNaHe exciplexes do not manifest such remarkable properties. The observations can be largely explained by assuming that the interaction of Na* with the helium nanodroplet can be described by the sum of Na*He pair potentials.

9:24AM A26.00006 Photoelectron imaging of doped helium nanodroplets, DANIEL NEUMARK, University of California, Berkeley — Photoelectron images of helium nanodroplets doped with Kr and Ne atoms are reported. The images and resulting photoelectron spectra were obtained using tunable synchrotron radiation to ionize the droplets. Droplets were excited at 21.6 eV, corresponding to a strong droplet electronic excitation. The rare gas dopant is then ionized via a Penning excitation transfer process. The electron kinetic energy distributions reflect complex ionization and electron escape dynamics.

9:36AM A26.00007 High Resolution Fluorescence Excitation and Dispersed Emission Spectra of Organic Molecules in Superfluid Helium Nanodroplets1, MARCEL DRABBELS — We present a theoretical study on the effect of a helium nanodroplet environment on the fragmentation dynamics of embedded rare gas cluster ions. As a complement to the fluorescence excitation spectrum the emission spectra provide important details on dynamic processes of intramolecular as well as intermolecular nature. This will be demonstrated for various examples such as intramolecular proton tunnelling, isomeric van der Waals complexes, tautomerization and microsolvation.

1A Humboldt fellowship for A.V. is gratefully acknowledged

9:48AM A26.00008 Coherent boson dynamics in strongly localized potentials - helium excitations at planar aromatic molecules and trapped cold atoms, K. BIRGITTA WHALEY, University of California, Berkeley — Planar aromatic molecules provide strongly localizing potentials for helium that considerably modify the local superfluid properties of a solvating helium environment. I shall describe some of the effects of these interactions on the solvation structure and spectroscopy of tetracene and phthalocyanine in helium droplets, comparing results of zero and finite temperature quantum Monte Carlo simulations with experimental data. The helium atoms closest to the molecule are seen to show similarities to trapped cold atoms in multi-well potentials. Studies of cold bosons with attractive and repulsive interactions in double well potentials will also be presented, showing formation of squeezed and quantum superposition states of cold atoms.

10:24AM A26.00009 Fragmentation dynamics inside helium nanodroplets: new theoretical results, NADINE HALBERSTADT1, LCAR-IRSAMC, CNRS and Universite Toulouse, DAVID BONHOMMEAU2, University of Minnesota, MARIUS LEWINERZ3, Universite Paris Est, Laboratoire de Chimie Theorique — We present a theoretical study on the effect of a helium nanodroplet environment on the fragmentation dynamics of embedded rare gas cluster ions. The helium atoms are treated explicitly, with zero-point effects taken into account through an effective helium-liquid interaction potential. All the nonadiabatic effects between electronic states of the ionized gas cluster are taken into account. Our results reveal new mechanisms for the cooling by helium, and show that the dopant can be ejected from the helium droplet. These results will be presented and discussed.

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10:36AM A26.00010 Suppressing the fragmentation of fragile molecules in helium nanodroplets by co-embedding with water: Possible role of the electric dipole moment, YANFEI REN, VITALY KRESIN, University of California, Berkeley — When fragile molecules are embedded in liquid helium nanodroplets, electron-impact ionization usually leads to fragmentation which is as extensive as for isolated gas-phase molecules. This occurs because of the energy release accompanying charge transfer from the impurity to the He+ hole created by electron bombardment. However, in experiments with glycin, polyglycine peptide chains, and alkan hydrocarbon chains we found that if a few molecules of water are co-embedded with these molecules, the fragmentation of the latter is drastically reduced or completely eliminated. On the other hand, the fragmentation of alkanethiols remains unaffected. On the basis of these observations, it is proposed that the fragmentation “buffering” effect may correlate with the magnitude of the impurity’s electric field and the ionization of the He+ hole through the droplet.

1Supported by NSF

10:48AM A26.00011 Path integral investigation of the electronic spectra of He-tetracene clusters, HEATHER D. WHITLEY1, Lawrence Livermore National Laboratory, Livermore, CA 94551, K. BIRGITTA WHALEY, Department of Chemistry and Kenneth S. Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720 — Planar aromatic molecules (PAMs) are nanoscale precursors to bulk graphite. Their electronic spectra have been extensively studied in He nanodroplets and show a number of unusual spectroscopic features. We have conducted many-body quantum simulations of tetracene in He nanodroplets to probe the 1.1 cm−1 spectral splitting of the electronic origin seen for this PAM. We calculate spectral shifts and He density profiles via path integral quantum Monte Carlo simulations. The spectral splitting is examined using a path integral correlation function approach to determine the lowest-lying vibrational excitation frequencies for small HeN−tetracene clusters. Simulations in the $S_1$ state of tetracene utilize a semi-empirical perturbative interaction potential for a He atom with a PAM. Results for the splitting of the electronic origin and the spectral shifts are in good agreement with experiment. Prepared by LLNL under Contract DE-AC52-07NA27344.

1Previous affiliation: Department of Chemistry and Kenneth S. Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720
8:00AM A27.00001 Low temperature spin dynamics and high pressure effects in frustrated pyrochlores, ISABELLE MIREBEAU, Laboratoire Léon Brillouin CEA/CNRS, CE-Saclay, 91919 Gif sur Yvette France — Frustrated pyrochlores R2MoO7, where R is a rare earth and M+4 a transition or sp metal ion, show a large variety of exotic magnetic states due to the geometrical frustration of the pyrochlore lattice, consisting of corner sharing tetrahedra for both R and M ions. Neutron scattering allows one to measure their magnetic ground state as well as the spin fluctuations, in a microscopic way. An applied pressure may change the subtle energy balance between magnetic interactions, inducing new magnetic states. In this talk, I will review recent neutron results on Terbium pyrochlores, investigated by high pressure neutron diffraction and inelastic neutron scattering.

8:36AM A27.00002 Spin Structure of Three Dimensional Frustrated Magnetic System of Tb2Mo2O7 — DEEPAK SINGH, JOEL HELTON, Massachusetts Institute of Technology, JEFFREY LYNN, NCNR, National Institute of Standard and Technology. YOUNG LEE, Massachusetts Institute of Technology, YOUNG LEE TEAM, JEFFREY LYNN COLLABORATION — The pyrochlore compound Tb2Mo2O7 has been of interest since it exhibits spin-glass behavior despite the apparent lack of chemical disorder. This compound crystallizes in a cubic space group in which both the Tb and Mo atoms form three-dimensional networks of corner-sharing tetrahedra. Thus, each magnetic ion resides on a highly frustrated pyrochlore lattice. To clarify the nature of the spin correlations in the spin-glass state of Tb2Mo2O7, we have succeeded in growing single crystal samples. Magnetic susceptibility (zero field cooled and field cooled) measurements confirm the spin-glass behavior, similar to that observed in previous powder samples. Recently we performed elastic neutron scattering measurements on a single crystal sample and identified the Q-vectors associated with the short-range diffuse scattering. The spin structure for this compound, consistent with elastic scattering, will be discussed. In addition, recent inelastic neutron scattering measurements will be discussed.

8:48AM A27.00003 Field driven phases in the geometrically frustrated dipolar Heisenberg pyrochlore antiferromagnet Gd4Ti2O7, MATTHEW ENJALRAN, Department of Physics, Southern CT State University, New Haven, CT, ADRIAN DEL MAESTRO, Department of Physics, Harvard University, Cambridge, MA, MICHEL J.P. GINGRAS, Department of Physics and Astronomy, University of Waterloo, Waterloo, ON, Canada; Canadian Institute for Advanced Research, Toronto, ON, Canada — The rare-earth pyrochlore gadolinium titanate, Gd4Ti2O7, represents an excellent experimental realization of a Heisenberg antiferromagnet (AFM) in a frustrated geometry with weak long-range dipole-dipole interactions (approximately 20% of nearest neighbor AFM exchange). Experiments on Gd4Ti2O7 in a magnetic field reveal a complex phase diagram associated with the breaking of spatial symmetries of the pyrochlore lattice as the field is applied along select symmetry directions. We study a model of classical Heisenberg spins (O(3) symmetry) on a pyrochlore lattice with exchange and dipolar interactions within mean-field theory. We report recent single crystal neutron scattering measurements of the XY pyrochlore antiferromagnet Er3Ti2O7 in zero and non-zero magnetic field applied along the (110) direction. Previous results show a magnetically-ordered ground state which is suggested to be stabilized by an unusual order-by-disorder mechanism driven by quantum fluctuations [1]. We present measurements of the low-lying spin excitations of this system, revealing Goldstone modes previously thought to be absent. [1] J.D.M. Champion et al. “Er3Ti2O7: Evidence of quantum order by disorder in a frustrated antiferromagnet” PRB 68 (2003)
HEINZ, Columbia University — Single-walled carbon nanotubes (SWCNTs) constitute a fascinating class of 1-dimensional materials. While the electrical, thermal, and mechanical properties of SWCNTs have been studied in depth for some time, only recently have their optical properties emerged as a major topic of research. This interest reflects several factors: The importance of nanotube optical properties for analysis of their structure, quality, and growth; the potential to use their optical properties to control and integrate electronic and optical functions; and the unique properties of optical excitations such as the hundreds of electronic states available in each nanotube. 

We will present an overview of our current understanding of excited electronic states in nanotubes and of the methods and applications of single-molecule optical spectroscopy of carbon nanotubes. We will present recent results on optical spectroscopy of single carbon nanotubes, and compare these results with theoretical predictions. These results will be presented and compared with relevant theoretical studies.

1 C. E. Shannon, Bell System Technical Journal, 27, 379 (1948)

We acknowledge the financial support from NSF grant DMR-0353610 and R.S.F. thanks CNPq-Brazil for sponsorship.
weakly-dispersive low-energy (quasi-1D absorbing bodies [1]. We show that these interactions result in the exciton-plasmon coupling that is significant in its strength due to the presence of modes of a single-walled carbon nanotube. We use our previously developed Green's function formalism to quantize an electromagnetic field in the presence of University, KEVIN TATUR, LILIA WOODS, University of South Florida — We study theoretically the interactions of excitonic states with surface electromagnetic

9:12AM A28.00003 Effective One-Dimensional Electron-Hole Interaction in Single-Walled Carbon Nanotubes1, JACK DESLIPPE, MARIO DIPOPPA, UC Berkeley and LBNL, DAVID PRENDERGAST, Molecular Foundry, LBNL, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro, STEVEN LOUIE, UC Berkeley and LBNL — Using the results of ab initio GW-Bethe-Salpeter-Equation (GW-BSE) calculations on the excitonic effects in single-walled carbon nanotubes (SWCNTs), we derive a 1D quantum model for the electron-hole interaction in both semiconducting and metallic SWCNTs. The model includes the important effects of spatial dependent screening and reproduces the exciton binding energies and envelope wave functions of the complete GW-BSE solution of the electron-hole excited states. The inclusion of the spatial dependence in the dielectric function arises from the effects of the surrounding tube on the density of states. The model captures the positioning of the exciton states in the spectrum whose calculated energies differ dramatically from those obtained using previous models based on constant dielectric screening. The present effective interaction can be used to calculate the binding energies of exciton states in a range of SWCNTs, which would be impractical by ab initio study.

9:24AM A28.00004 Environmental effect for exciton transition energy of single carbon nanotubes1, RICHIRO SAITO, KENTARO SATO, PARK JINSUNG, Tohoku University, YUHEI MIYAUCHI, SHIGEO MARUYAMA, The University of Tokyo, MILDRED DRESSELHAUS, GENE DRESSELHAUS, MIT — The exciton transition energies of nanotube samples which are observed in resonance Raman, photo-absorption, and photoluminescence spectroscopies, depend on the surrounding materials (environmental effect). The environmental effect can be explained by screening of the excitonic states by the dielectric materials. We calculate the transition energies for many different (n,m) carbon nanotubes up to 4eV and to 3nm in diameter. The calculated results are compare with many experimental data with different conditions for samples. The energy shift for the exciton transition energies can be explained by using a fitting parameter of static dielectric constants of surrounding materials. However we will show that the effective dielectric constant has a unique, type, metallicity, diameter, and energy dependence of the dielectric constants in order to reproduce the exciton energies for the wide range of diameter and excitation energies. By analyzing the data, we will give a simple formula for the dielectric constants for carbon nanotubes themselves and the surrounding materials as a function of chirality and diameter of single wall carbon nanotubes.

9:36AM A28.00005 Surface Exciton-Plasmons in Carbon Nanotubes1, IGOR BONDAREV, NC Central University, KEVIN TATUR, LILIA WOODS, University of South Florida — We study theoretically the interactions of excitonic states with surface electromagnetic modes of a single-walled carbon nanotube. We use our previously developed Green’s function formalism to quantize an electromagnetic field in the presence of quasi-1D absorbing bodies [1]. We show that these interactions exhibit a new plasmon coupled exciton bands that is sensitive to the presence of weakly-dispersive low-energy (~0.5-2eV) interband surface plasmon modes [2] and large exciton excitation energies ~1eV in small-diameter nanotubes [3]. We estimate the exciton-plasmon Rabi splitting to be ~0.01-0.1eV which is close to that observed in organic semiconductors [4] and much larger than that reported for hybrid semiconductor-metal nanoparticle molecules [5]. We calculate the exciton absorption line shape and demonstrate a clear line splitting effect as the exciton energy is tuned to the closest interband surface plasmon resonance.

9:48AM A28.00006 Cross-polarized optical absorption of single-walled carbon nanotubes probed by photoluminescence excitation spectroscopy, UV-Vis-IR and polarized Raman Scatterings , SHIGEO MARUYAMA, The University of Tokyo — Because of the depolarization effect, or so-called antenna effect, optical absorption of single-walled carbon nanotubes (SWNTs) is weak when excited by light polarized perpendicular to the nanotube axis. However, in photoluminescence (PL) excitation spectra of isolated SWNTs, PL peaks due to cross-polarized excitation can be clearly identified. By decomposing the cross-polarized component, the optical transition energy of E12 or E21 can be experimentally measured, and the smaller exciton binding energy for perpendicular excitations is concluded [1]. Cross-polarized absorption is dominant in the absorption of a vertically aligned film of SWNTs [2] when excited from the top of the film. In our previous study, a p-plasmon absorption at 5.25 eV was revealed in contrast to 4.5 eV for parallel excitation [3]. Resonant Raman scattering from such a film is also influenced by the cross-polarized excitation [4]. Even though a Kataura plot for the E33 and E44 range has been proposed by using such a vertically aligned film [5], polarized Raman scattering excitation energy is tuned to the closest interband surface plasmon resonance.

References:

10:24AM A28.00007 Carbon nanotube excited states: the role of the environment , PHAEDON AVOURIS, IBM T.J. Watson Research Center — The nature of the excited states and the radiative and non-radiative decay of isolated CNTs will be briefly reviewed. I will then focus on the role of the environment, external fields and photon confinement on these properties. I will discuss the use of photovoltage microscopy as a means of imaging environment-induced potential fluctuations in CNTs, presence and size of Schottky barriers at contacts and the extent of band-bending. Scanning resonant micro-Raman scattering will be used to evaluate the CNT excited state shifts induced by the substrate, and, also, the phonon frequency and linewidth changes due to the effects of trapped substrate charges, and charge-transfer effects. Variations in local charge density will be determined by making use of the dependence of electron-phonon coupling on the local charge density. The non-radiative decay of free and localized excitons will then be examined and it will be shown that a phonon-assisted electronic decay mechanism made possible by interaction with the environment can dominate the lifetime of excited CNTs. Finally, results on the modification of the radiative properties of CNTs by changing the photon field mode density for CNTs enclosed in micro-cavities will be presented.

Monday, March 10, 2008 8:00AM - 11:00AM –
Session A29 DMP: Focus Session: Carbon Nanotubes and Related Materials I: Graphene Transport
Morial Convention Center 221

8:00AM A29.00001 Thermopower of Few-Layer Graphene Devices , PENG WEI, WENZHONG BAO, YONG PU, CHUN NING LAU, JING SHI — We report thermopower measurements of few-layer graphene (FLG) devices at low temperatures. FLG flakes are separated by mechanical exfoliation and then connected to form devices using electron beam lithography. FLG devices are fabricated on a 300 nm-thick SiO2 layer which separates from the heavily-doped silicon substrate used as a gate. As the gate voltage is swept from -55 V to 55 V, the electrical conductivity of FLG devices undergoes a minimum. In the meantime, the Seebeck coefficient changes the sign near the conductivity minimum, marking the transition from p- to n-type in graphene. By directly comparing the derivative of the logarithmic conductivity with the measured Seebeck coefficient, we have experimentally validated the Mott relation. We also have measured the Seebeck coefficient and electrical conductivity under magnetic fields up to 8T. Detailed analysis of the experimental data will be presented.

8:12AM A29.00002 Measurement of the Thermal Conductance at the Graphene-Quartz Interface by Optical Pump-Probe Spectroscopy , CHUN HUNG LUI, KIN FAI MAK, YANG WU, TONY HEINZ, Columbia University — We have determined the interfacial thermal conductance of single and multi-layer graphene samples prepared on quartz substrates by mechanical exfoliation of graphite. The measurements were performed by suddenly heating the graphene sample with a femtosecond optical laser pulse and then monitoring the sample’s subsequent temperature evolution through the slight changes in reflectivity experienced by a time-delayed optical probe pulse. For the study of thermal transport, the transient response occurring on a time scale of tens of picoseconds was relevant. A faster transient related to non-equilibrium electronic excitation was also observed at early delay times. By studying the dependence of the slow decay component on the number of graphene layers in the sample, we could identify interfacial heat flow as the relaxation mechanism. An interfacial conductance in excess of 5,000W/cm × K on the surface of graphene based-devices which are otherwise devoid of any surface adsorbates [2] in ultra high vacuum environment. Adsorbed potassium decreases the charge carrier mobility, renders the gate-dependent conductivity linear, shifts the minimum conductivity point in gate voltage, broadens the width of minimum conductivity region, and lowers the minimum conductivity. Our results are in qualitative agreement with a recent Boltzmann transport calculation [3]. New features, such as asymmetric response of electron-hole mobility and the observation of a “residual” conductivity (the extrapolation of the linear gate-voltage dependent conductivity to the minimum conductivity point) near 2 e2/h, indicate transport properties beyond the simple Boltzmann picture. [1] J.H.Chen et al., http://xxx.lanl.gov/abs/0708.2408. [2] M.Ishigami et al., Nano Letters, 7, 1643 (2007). [3] S. Adam et al., PNAS 104, 18392 (2007).

8:24AM A29.00003 A graphene-based atomic-scale switch , BRIAN STANDLEY, MARC BOCKRATH, California Institute of Technology — Graphene’s remarkable mechanical and electrical properties combined with its compatibility with existing planar CMOS technology make it an attractive material for novel computing devices. Thus far work has focused primarily on realizing transistor functionality. To complement this effort, we have developed a graphene-based switch that realizes a non-volatile memory element. Our devices have demonstrated tens of thousands of writing cycles and long retention times. Additionally, the devices’ atomic-scale dimensions correspond to bit densities far greater than present-day memory technologies. We will present the fabrication process, switching behavior, and further performance characterization.

8:36AM A29.00004 Electronic properties of graphene , KOSTYA NOVOSELOV, University of Manchester — Graphene is a first two-dimensional atomic crystal. In my talk I’ll overview our latest results on the electronic properties of this material.

9:12AM A29.00005 Charged Impurity Scattering in Graphene , MASA ISHIGAMI, JIANHAO CHEN, C. JANG, E.D. WILLIAMS, M.S. FUHRER, Physics Department, Materials Research and Engineering Center, and Center for Nanophysics and Advanced Materials, University of Maryland, College Park — We have measured the impact of charged impurity scattering on the transport properties of graphene sheets [1]. We vary the density of adsorbed potassium atoms in our experiment up to 5 × 1012 K/cm2 on the surface of graphene based-devices which are otherwise devoid of any surface adsorbates [2] in ultra high vacuum environment. Adsorbed potassium decreases the charge carrier mobility, renders the gate-dependent conductivity linear, shifts the minimum conductivity point in gate voltage, broadens the width of minimum conductivity region, and lowers the minimum conductivity. Our results are in qualitative agreement with a recent Boltzmann transport calculation [3]. New features, such as asymmetric response of electron-hole mobility and the observation of a “residual” conductivity (the extrapolation of the linear gate-voltage dependent conductivity to the minimum conductivity point) near 2 e2/h, indicate transport properties beyond the simple Boltzmann picture. [1] J.H.Chen et al., http://xxx.lanl.gov/abs/0708.2408. [2] M.Ishigami et al., Nano Letters, 7, 1643 (2007). [3] S. Adam et al., PNAS 104, 18392 (2007).

9:42AM A29.00006 Conductivity and Fano factor in disordered graphene , EDUARDO R. MUCCIOLI, Department of Physics, University of Central Florida, MI presente Department of Physics, University of Central Florida.

9:42AM A29.00007 The conductivity of pure graphene , SUBIR SACHDEV, LARS FRITZ, Harvard University, JOERG SCHMIALAN, Iowa State University — Pure graphene, in the absence of impurities or bias voltage, is described by a theory of Dirac fermions with Coulomb interactions. We argue that this theory has a finite conductivity, σ, and show that at frequencies ω ≪ k_B T/h (where T is absolute temperature) σ = Ξ(2e^2/h)/(ln(W/T))^2, where W is the bandwidth, and ξ is a universal number. We compute Ξ by the solution of a quantum Boltzmann equation. The influence of a dilute concentration of impurities and finite bias voltage is also discussed.
9:48AM A29.00008 Theoretical study of graphene transport regimes, SHAFFIQUE ADAM, S. DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park, MD 20742-4111, USA — In recent work [Adam et al. Proc. Natl. Acad. Sci. 104, 18392 (2007); Y.-W. Tan et al. arXiv:0707.1807, Phys. Rev. Lett., in press (2007)], we argued that the transport properties of currently available experimental graphene samples are dominated by diffusive carriers scattering off Coulomb impurity centers typically located in the substrate. In the current paper we study graphene monolayers, bilayers and nanoribbons and show theoretically that by tuning external parameters, one can access several different transport regimes ranging from the aforementioned diffusive Boltzmann transport to phase-coherent ballistic transport to classical percolation through puddles of electrons and holes. This work is supported by U.S. ONR and NRI-NSF.

10:00AM A29.00009 Impact of physisorbed species on transport properties of graphene, CHAUN JANG, JIANHAO CHEN, SHUDONG XIAO, Department of Physics and Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, MASA ISHIHIGAMI, ELLEN WILLIAMS, Department of Physics and Materials Research Science and Engineering Center, University of Maryland, College Park, MD 20742, MICHAEL FUHRER, Department of Physics and Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742 — We have measured the impact of physisorbed species, including Argon, Krypton, Nitrogen, water and Benzene, on the transport properties of mechanically-exfoliated graphene sheets on SiO$_2$/Si in an ultra-high vacuum environment at temperatures near 30 K. We controlled the gas dosage down to the sub-monolayer level and found species-specific effects on the field-effect mobility of graphene. We observed the influence of different molecular sizes, molecular dipole moment, and intermolecular interactions. We will discuss our results in the context of recent theoretical calculations within the Boltzmann transport framework.

1 Supported by ONR N000140610882, NSF CCF-06-34321 (MSF), NSF-UMD-MRSEC DMR 05-20471 and the MI is supported by the DCI Postdoctoral Fellowship program.

10:12AM A29.00010 Stress-induced Controlled Fabrication of Graphene Nano Ribbons and Carbon Nanotubes via Electrostatic force and electrical transport properties of freely suspended graphene monolayers and bi-layers, ANTON SIDOROV, DAVID MUDD, VLADIMIR DOBROKHOTOV, C.S. JAYANTHI, SHI-YU WU, GAMINI SUMANASEKERA — A simple electrostatic force to transfer loosely bound graphene sheets from a freshly cleaved highly oriented pyrolytic graphite (HOPG) to a desired substrate has been recently reported (Sidorov et al., Nanotechnology, 2007). Here we demonstrate that this technique can be further extended to roll/scroll graphene sheets in a controllable manner by changing the environment during this electrostatic deposition. Deposition under high vacuum (10$^{-7}$ Torr) is observed to deposit extremely flat graphene monolayers on a substrate. In contrast, high density of completely scrolled graphene layers are observed in hydrogen atmosphere and in the presence of an electrostatic field. No scrolling was seen in He atmosphere; but partial scrolling is seen in nitrogen atmosphere under the influence of an electrostatic field. It is believed that in addition to the stress induced due to the adsorption of hydrogen, an additional electrostatic field is necessary to scroll the graphene layers loosely bound to HOPG. Also electrical transport properties of monolayers and bi-layers of graphene layers freely suspended between two electrodes and deposited between trenches on a substrate will be presented and compared.

10:24AM A29.00011 Interaction of Si atoms and Si-based radicals with carbon nanotubes and graphene monolayers, KISEOK CHANG, SAVAS BERBER, DAVID TOMÁNEK, Michigan State University — We use ab initio density functional calculations to study the interaction of Si atoms and Si-based radicals, such as SiH$_3$, with single-wall carbon nanotubes and graphene monolayers. We find that both Si atoms and radicals form a strong chemisorption bond, accompanied by a small relaxation and a locally increased sp$^3$ bond character of the graphitic nanostructure. We identify the optimum adsorption geometries at different adsorbate coverages and adsorbate-related changes in the electronic structure and vibration spectra of the systems. We propose that successful functionalization of carbon nanotubes or graphene by Si atoms or Si-based radicals can be verified by studying changes in the radial breathing mode of nanotubes and the G-band of graphitic nanocarbons using Raman spectroscopy.

1 Supported by NSF NSEC Grant No. 425826.

10:36AM A29.00012 First-principles Studies of Metal Adsorption on Graphene, KEVIN T. CHAN, Department of Physics, University of California, Berkeley, J. B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, MARVIN L. COHEN, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — Quantitative first-principles theory can aid in understanding many experimental phenomena involving metal adsorption on graphene and carbon nanotubes, including adatom mass transport, modification of electronic, mechanical, and magnetic properties, and adhesion and efficacy of electrical contacts. In this work, the binding energy and geometry, charge transfer, work function, and electronic structure of adatom-graphene systems are calculated using first-principles density functional theory for a variety of metal elements. Trends in these calculated data are analyzed, and their implications for graphene-based devices are discussed.

1 This work was supported by National Science Foundation Grant No. DMR07-05941 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources were provided by Indiana University, SDSC, NERSC, and the Molecular Foundry.

10:48AM A29.00013 Carbon-based ion and molecular channels, KYAW SINT, BOYANG WANG, PETR KRAL, University of Illinois at Chicago, PROF. KRAL'S RESEARCH GROUP TEAM — We design ion and molecular channels based on layered carboneous materials, with chemically-functionlialized pore entrances. Our molecular dynamics simulations demonstrate that these ultra-narrow pores, with diameters around 1 nm, are highly selective to the charges and sizes of the passing (Na$^+$ and Cl$^-$) ions and short alkanes. We demonstrate that the molecular flows through these pores can be easily controlled by electrical and mechanical means. These artificial pores could be integrated in fluidic nanodevices and lab-on-a-chip techniques with numerous potential applications.

8:00AM A30.00001 First-principles calculations of zigzag-edge graphene nanostrips with different edge species, JOHN W. MINTMIRE, Oklahoma State University, DANIEL GUNLYCKE, Naval Research Laboratory, JUNWEN LI, Oklahoma State University, CARTER T. WHITE, Naval Research Laboratory — First-principles calculations have suggested that zigzag-edge graphene nanostrips terminated with hydrogen atoms have edge states which exhibit magnetic behavior. However, it is not clear that zigzag-edge graphene nanostrips terminated with other atoms or functional groups also show similar magnetic behavior. Our local-spin-density calculations suggest that some zigzag-edge nanostrips, including oxygen-terminated nanostrips, have no magnetic edges. One reason could be that there is charge transfer at the edges which effectively dopes the p-orbital network, causing the spin polarization to collapse.

1 This work was supported by the NRC and ONR through NRL, and at OSU by the DOE EPSCoR program.
8:12AM A30.00002 Hydrogenation of graphitic nanocarbons1, SAVAS BERBER, DAVID TOMAÑEK, Michigan State University, EUNJA KIM, PHILIPPE F. WÆCK, University of Nevada Las Vegas, GLEN P. MILLER, University of New Hampshire — We apply ab initio density functional calculations to study the hydrogenation of graphitic nanocarbons including fullerenes, onions and nanotubes using diethylenetriamine (DETA) as hydrogenation reagent. Our results indicate that transfer of atomic hydrogen from the amine end-group of chemisorbed DETA molecules to nanocarbons is an exothermic reaction. We explore the optimum pathway for the hydrogenation reaction and find the activation energy associated with sigmatropic rearrangement of chemisorbed hydrogen atoms to lie near 1 eV, thus facilitating formation of energetically favorable adsorbate structures by surface diffusion. Chemisorbed hydrogen assists in a local sp² to sp³ bonding conversion of the graphitic nanocarbons, causing large-scale structural changes ranging from local relaxations in nanotubes to shell opening in multi-wall onions.

1Supported by NSF NSEC Grant No. 425826.

8:24AM A30.00003 Electronic Structure Study of Edge Saturated Graphene Nanoribbons, YIMING ZHANG, PHILIP SHEMELLA, Rensselaer Polytechnic Institute, P.M. AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute, RENSESLEAER POLYTECHNIC INSTITUTE TEAM — Using density functional theory and GW method, we have studied how the electronic structures of graphene nanoribbons responds to the edge saturation. The energy gaps and effective mass of the nanoribbons are highly sensitive to the edge states, as well as the nanoribbon width. This suggests a new approach to modify the electronic structure of graphene nanoribbons by tweaking the edge saturation.

8:36AM A30.00004 Imaging massless Dirac fermion flow in graphene nanoribbons, LIVIU P. ZĂRBO, Texas A&M University, BRANISLAV K. NIKOLIC, University of Delaware — Since its recent experimental discovery, graphene has been the focus of intense theoretical and experimental research. Its unconventional electronic structure characterized by the linear momentum dispersion of electrons which behave as massless Dirac particles at half-filling makes graphene an ideal candidate not only for investigating fundamental physics questions, but also for constructing new nanoscale devices. Despite its importance for device applications, there are very few studies of local features of electronic transport in graphene nanoribbons (GNRs). Moreover, the application of recently advanced scanning probe techniques to imaging electronic flow in graphene is expected to lead to many interesting discoveries. Therefore, we investigate the local features of charge transport through GNRs, by employing our bond current formalism which expresses the local current fluxes flowing between neighboring sites of the hexagonal lattice in terms of nonequilibrium Green functions. We show that, while the charge density profiles for clean zigzag graphene nanoribbons (ZGNRs) close to Dirac point peak at the edges due to the zero-energy edge states, the current densities concentrate towards the nanoribbon center. The analysis of local charge current flow explains unusual transport properties of ZGNRs such as low sensitivity of current flow to edge vacancies or long-range impurities. Journal Ref: EPL 80, 47001 (2007).

8:48AM A30.00005 First principles study of graphene nanoribbons and nanorectangles, PHILIP SHEMELLA, LI CHEN, YU ZHOU, YIMING ZHANG, SREEKALA SUBBULAKSHMI, PULICKEL AJAYAN, SAROJ NAYAK, Rensselaer Polytechnic Institute — We have studied the finite size effect on the electronic structure of graphene nanoribbons (GNRs) using first principles density functional techniques. In particular, we have computed the energy gap dependence on the width and length for zero-dimensional nanoribbons for both the armchair and zigzag ribbons; and compared to the one-dimensional (infinite length) cases. One-dimensional armchair ribbons are expected to be metallic if the number of carbon atoms across the ribbon is N = 3M-1, and non-metallic N ≠ 3M-1, where M is an integer. In addition to quantum confinement along the width of the ribbon for metallic widths, an additional finite size effect emerges along the length of ribbons only for non-metallic armchair ribbons. The origin of additional quantum confinement in these structures is explained based on the energy states near the Fermi energy. The differences between zero- and one-dimensional electronic structure properties are considered with the addition of passivating groups and their effect on the electronic properties of graphene and their impact on nanoelectronics devices are discussed.

9:00AM A30.00006 Band gaps in armchair-edge graphene nanostraps1, CARTER T. WHITE, DANIEL GUNLYCKE, Naval Research Laboratory, JOHN W. MINTMIRE, Oklahoma State University — First-principles calculations have shown that all graphene nanostraps terminated with hydrogen atoms exhibit band gaps at the Fermi level. In the case of armchair-edge nanostraps, the calculations contradict a first-nearest-neighbor tight-binding prediction that one third of these nanostraps should be metallic. At the one-electron level, at least two independent causes for the band gaps in these nanostraps have been suggested, namely lattice distortion and long-range interactions. In this presentation, we present theoretical calculations of arbitrary armchair-edge nanostraps. The model, which includes distortion of edge atoms and third-nearest-neighbor interactions, leads to band gaps and band structures which are in good agreement with those obtained from our first-principles calculations.

1This work was supported by the NRC and ONR through NRL, and at OSU by the DOE EPSCoR program.

9:12AM A30.00007 Study of partial oxidation of zigzag graphene 1-d ribbons, S. SREEKALA, Y. ZHANG, P.M. AJAYAN, S.K. NAYAK, Rensselaer Polytechnic Institute — We study the effect of partial oxidation of graphene 1-d ribbons using the first principle- density functional theory. We have considered zigzag graphene, n=8 with four dangling carbon on each edge. The zigzag graphene 1-d ribbon is a zero bandgap material, when it is functionlialized completely with hydrogen atoms. However, when two of these hydrogen atoms are replaced by oxygen, the band gap opens. This is due to the fact that the oxygen forms double bond with the carbon and hence disrupts the delocalization of the π and π* bond. This functionalization does not induce magnetization. On further increase of oxygen, the band decreases. When oxidation is more than 75% on one side of the graphene ribbon or on either sides, the lone pair of electrons of the oxygen induces magnetization to some of the carbon atoms. Also some configurations of partially oxidized graphene show that antiferromagnetic order is the stable ordering in these systems.

9:24AM A30.00008 Graphene Nanoribbon(GNR) based Nanoelectronics for Interconnect Applications and Logic Devices using First Principles Calculations1, YU ZHOU, SUBBULAKSHMI SREEKALA, YIMING ZHANG, PHILIP SHEMELLA, Rensselaer Polytechnic Institute, PULICKEL AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute, RPI TEAM — We have studied electronic structures of graphene ribbon based nanoelectronics using first principles density functional techniques for interconnect applications as well as for logic devices. The conductance behaviors of them are computed based on Non-equilibrium Green’s Function. For example, we have calculated the energy gap and I-V curve of Schottky diode built by connecting two zig-zag GNRs with different passivations. All new configurations will show nonlinear I-V behavior and explicit step feature is observed in the I-V plot as well. There is also a small charge transfer at the junction area for this new configuration which is more like a traditional diode, which leads to different phenomena during the negative biasing.

1Interconnect Focus Center
Studies on such interfaces. It is not completely clear yet to what extent they are decisive for some of these properties. In this talk I will discuss recent experimental and theoretical results. They can become conducting, remain insulating, show magnetic activity and even become superconducting. An important aspect concerns the role of oxygen vacancy effects. In the case of voids in semiconductor ribbons, we study the magnetism associated to a single void and the magnetic interactions developed between them.[2] [1] J. Fernández-Rossier, J. J. Palacios, Phys. Rev. Lett. 95, 226801 (2005). [2] M. Zarea and N. Sandler, Phys. Rev. Lett. Dec (2007)

Ab-initio calculation of bonding, charge redistribution and transfer of graphene on amorphous silica, NING SHEN, JORGE SOFO, Department of Physics, Penn State University — We study the effects of an amorphous silica substrate on the electronic structure and electron density of graphene using Density Functional Theory. We observe that the silica substrate transfers charge to the graphene layer and the workfunction of the combined system is lower than that of an isolated graphene sheet. The inhomogeneous charge distribution of the substrate induces an inhomogeneous charge redistribution on the graphene layer, which is experimentally observed as electron and hole puddles. The binding energy between one graphene layer and the substrate is weak and reveals no sign of chemical bonding. This can also be inferred from a rigid band shift observed in the system.

Electron states of mono- and bilayer graphene on SiC probed by STM, FRANÇOIS VARCHON, PIERRE MALLET, CÉCILE NAUD, Institut NEEL CNRS/UJF, 25 rue des Martyrs BP166, 38042 Grenoble, CLAIRE BERGER, The Georgia Institute of Technology, Atlanta, Georgia 30332-0430; Institut NEEL CNRS/UJF, 25 rue des Martyrs BP166, 38042 Grenoble, LAURENCE MAGAUD, JEAN-YVES VEUILLEN, Institut NEEL CNRS/UJF, 25 rue des Martyrs BP166, 38042 Grenoble — We present a scanning-tunneling microscopy (STM) study of a gently graphitized 6H-SiC(0001) surface in ultrahigh vacuum [1]. From an analysis of atomic scale images, we identify two different kinds of atomic scale contrasts, which we attribute to mono- and bilayer (or trilayer) graphene capping a C-rich interface. At any temperature, both terraces show quantum interference effects generated by point defects. Such interferences are a fingerprint of π-like states close to the Fermi level. We conclude that the metallic states of the first graphene layer are almost unperturbed by the underlying interface, in agreement with recent ab initio studies [2] and photoemission experiments [3]. However, a significant density of interface states is detected close to the Fermi level in the C-rich interface. [1] P. Mallet et al., Phys. Rev. B 76, 041403(R) (2007) [2] F. Varchon et al., Phys. Rev. Lett. 99, 126805 (2007) [3] A. Bostwick et al., Nat. Phys. 3, 36 (2007)

Magnetism in graphene nanoislands and nanovoids, JUAN JOSE PALACIOS, JOAQUIN FERNANDEZ-ROSSIER, Universidad de Alicante, LUIS BREY, ICM-M-CSC — The rules to predict the magnetic state of both graphene nanoislands and nanovoids in otherwise perfect graphene systems are presented. We discuss how the shape of the island or void, the associated imbalance in the number of atoms belonging to the two graphene sublattices, the existence of zero-energy states, and the total and local magnetic moment are intimately related. We consider electronic interactions both in a mean-field approximation of the one-orbital Hubbard model and with density functional calculations. The magnetic properties of nanometer-sized graphene structures with triangular and hexagonal shapes terminated by zigzag edges happen to be drastically different[1]. In the case of voids in semiconductor ribbons, we study the magnetism associated to a single void and the magnetic interactions developed between them[2]. [1] J. Fernández-Rossier and J. J. Palacios, Phys. Rev. Lett. 99, 177204 (2007). [2] J. J. Palacios,J. Fernández-Rossier, L. Brey, in preparation.

The electronic structure of graphene layers on SiO2 substrate, YONG-JU KANG, JOONGOOK KANG, KEE JOO CHANG, Korea Advanced Institute of Science and Technology — Graphene is a single layer of carbon atoms packed in a honeycomb lattice, and its quasiparticles behave like massless Dirac fermions. Since graphene is usually supported and deposited on dielectric materials such as SiO2 and SiC, interactions between graphene and substrate atoms can modify the electronic structure of graphene. In this work we study the structural and electronic properties of a few graphene layers on SiO2 surfaces through first-principles calculations within the local-density-functional approximation. We examine interactions between graphene layers and Si- and O- terminated surfaces of α-quartz and the substrate-induced doping effect. For a single graphene layer, we find that graphene strongly interacts with the O-terminated surface. A charge transfer occurs from the graphene to the surface O atoms, leading to the p-type doping. For a bilayer graphene in AB stacking, the charge transfer mostly occurs for the graphene layer right on the substrate, resulting in an asymmetric distribution of electron charges between two graphene layers and thus a gap opening at the Dirac point.

Pair condensation in electron-hole graphene bi-layer, RAFI BISTRITZER, HONGKI MIN, JUNG-JUNG SU, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin — Using self consistent Hartree Fock calculations we show that an electron-hole graphene bi-layer exhibits spontaneous interlayer coherence when the distance between layers is sufficiently small. We describe the unique transport properties of the emergent dipolar superfluid and relate them to the nature of the underlying massless Dirac particles.
8:36AM A31.00002 Magnetic anisotropy modulation in Fe$_3$O$_4$/BaTiO$_3$(100) epitaxial structures, C.A.F. VAZ, J. HOFFMAN, A. POSADAS, C.H. AHN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University, New Haven, CT 06520 — Renewed interest in ‘classical’ ferroic materials has been accompanied by the study of a new class of multiferroic composite materials, based on magnetic and dielectric multilayer structures. One motivation is the search for materials that allow independent control of both the magnetic and electric properties. In this context, we investigate the modulation of the magnetic anisotropy of a 10 nm magnetite (Fe$_3$O$_4$) film grown epitaxially by off-axis magnetron sputtering on (001)BaTiO$_3$ (BTO). SQUID and magnetoresistance measurements as a function of temperature show a series of discontinuities that are attributed to changes in the strain of the magnetite film via elastic coupling with the substrate, as the latter undergoes a series of structural phase transitions. Magnetic hysteresis loops carried out at temperatures above and below each transformation in the BTO elucidate the variation of the effective anisotropy of the Fe$_3$O$_4$ film. The possibility of using the piezoelectric response of BTO to modulate the magnetic anisotropy of magnetite films is discussed.

8:48AM A31.00003 Epitaxial strain-mediated spin-state transitions: can we switch off magnetism?, JAMES RONDINELLI, NICOLA SPALDIN, Materials Dept., UC Santa Barbara, MATERIALS RESEARCH LABORATORY COLLABORATION — We use first-principles density functional theory calculations to explore spin-state transitions in epitaxially strained LaCoO$_3$. While high-spin to low-spin state transitions in minerals are common in geophysics, where pressures can reach over 200 GPa, we explore whether heteroepitaxial strain can achieve similar transitions with moderate strain in thin films. LaCoO$_3$ is known to undergo a low-spin ($S=0$, $t^6_2g^0$) to intermediate-spin ($S=1$, $t^5_2g^1$) or high-spin ($S=2$, $t^4_2g^2$) state transition with increasing temperature, and thus makes it a promising candidate material for strain-mediated spin transitions. Here we discuss the physics of the low-spin transition and changes in the electronic structure of LaCoO$_3$, most notably, the metal-insulator transition that accompanies the spin-state transitions with epitaxial strain. As thin film growth techniques continue to reach atomic-level precision, we suggest this is another approach for controlling magnetism in complex oxide heterostructures.

9:00AM A31.00004 Density functional study of ferromagnetic ferroelectric LaMnO$_3$/BaTiO$_3$ superlattice, LEONARD KLEINMAN, BHAGAWAN SAHU, ADRIAN CIUCIVARA, University of Texas at Austin — Using the GGA + U density functional, we have calculated the lattice constants, atomic positions, magnetization, and ferroelectric polarization of a (LaMnO$_3$)$_n$(BaTiO$_3$)$_m$ superlattice containing five LaO and TiO$_2$ planes and four MnO$_2$ and BaO planes. Although LaMnO$_3$ is antiferromagnetic, it is ferromagnetic in the superlattice. An approximation to the ferroelectric polarization, obtained from a comparison of superlattice and bulk crystal atomic displacements and unit cell volumes, is found to agree reasonably well with the polarization obtained from a Berry phase calculation. The electric polarization points along the longer in-plane lattice vector, while the atomic spins, after the spin-orbit interaction and spin noncollinearity are included, are all in directions close to that lattice vector.

9:12AM A31.00005 Electron Localization and Interface Magnetism in CaRuO$_3$/CaMnO$_3$ Superlattices, J.W. FREELAND, Advanced Photon Source, Argonne National Lab., J. CHAKHALIAN, University of Arkansas, Fayetteville, J.J. KAVICH, Advanced Photon Source, Argonne National Lab., B. KEIMER, Max Planck Institute for Solid State Research, H.N. LEE, Oak Ridge National Lab. — We present a study of interface physics in superlattices composed of a G type anti-ferromagnetic insulator (CaMnO$_3$) and a paramagnetic metal (CaRuO$_3$). Using laser MBE, ultra-thin superlattices were grown with the structure [CaRuO$_3$ (N u.c.)/CaMnO$_3$ (10 u.c.)]$_6$ on LaAlO$_3$(100) substrates. Polarized x-ray probes clearly show a large Mn magnetic moment, which is attributed to a canted anti-ferromagnetic state at the interface. The electronic state of the system was probed by current-in-plane transport measurements. Due to the large resistivity of CaMnO$_3$, magneto-transport measurements probe primarily the behavior of the carriers in the CRO layer, which show a non-bulk like insulating behavior that is attributed to disorder induced localization from interface scattering. Field dependence shows a large negative magneto-resistance (MR), which results from strong scattering of the carriers by Mn spins at the interface since the MR drops with increasing CRO layer thickness. Work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. JC is funded by U.S. DOD-ARO under Contract No. 0402-17291.

9:24AM A31.00006 Exploring artificial layered heterostructures of LaM’O’3/LaM”O’3 (M’M” = NiCr, FeCr and NiV), J. LII, M. KAREEV, University of Arkansas, Fayetteville, J.W. FREELAND, Advanced Photon Source, Argonne National Lab., A. KAREEV, University of Arkansas, H.W. LEE, Oak Ridge National Lab. — Digital synthesis of atomically sharp interfaces between strongly correlated electron systems can provide a template to build completely new materials. Here we present our results on magnetism and electronic structure in LaM’O’3/LaM”O’3 (M’M” = NiCr, FeCr and NiV) superlattices by using polarized X-ray spectroscopies. Using laser MBE, the (111) and (100) oriented ultrathin superlattices were grown with alternating layer thicknesses of 1 unit cell. In the bulk, LaM03 (M=Cr,Fe,V) are antiferromagnetic insulators while LaNiO3 is a paramagnetic metal. The evolution of element specific magnetism and charge at the interface containing five LaO and TiO$_2$ planes and four MnO$_2$ and BaO planes. Although LaMnO$_3$ is antiferromagnetic, it is ferromagnetic in the superlattice. An approximation to the ferroelectric polarization, obtained from a comparison of superlattice and bulk crystal atomic displacements and unit cell volumes, is found to agree reasonably well with the polarization obtained from a Berry phase calculation. The electric polarization points along the longer in-plane lattice vector, while the atomic spins, after the spin-orbit interaction and spin noncollinearity are included, all point in directions close to that lattice vector.

9:36AM A31.00007 Strain effect on Magnetism at the Manganite Interfaces: SrMnO$_3$/LaMnO$_3$, BIRBARAB NANDA, SASHI SATPATHY, University of Missouri, Columbia — Recently it has been shown that new magnetic and electronic phases can be produced by varying the strain condition at the manganese interfaces[1]. From the density-functional studies of the electronic structure at the interface of SrMnO$_3$ and LaMnO$_3$ we show that the epitaxial strain, which enforces a tetragonal distortion, splits the itinerant interface Mn-$e_g$ states to $x^2-y^2$ and $3z^2-R_1$ states. If the strain is tensile in the plane the $x^2-y^2$ orbital becomes more occupied, enhancing thereby the ferromagnetic double exchange which overcomes the antiferromagnetic super exchange between the core $t_{2g}$ states to produce a net in-plane ferromagnetic interaction. Due to the lower occupancy of the $3z^2-R_1$ orbitals, the super exchange supercedes the double exchange to produce out-plane antiferromagnetic ordering. For in-plane compressive strain higher occupancy of $3z^2-R_1$ orbital results in the out-of-plane ferromagnetic ordering while in-plane ordering remains antiferromagnetic. Without any epitaxial strain, the itinerant $x^2-y^2$ and $3z^2-R_1$ states are more or less equally occupied and ferromagnetic ordering prevails both in-plane and out-of-plane. While for the tensile strain we find the heterostructure to be metallic, for the compressive strain an insulating phase is obtained if the strain is sufficiently large. This work was supported by DOE-DE-FG02-00ER45818.

9:48AM A31.00008 Asymmetric and modulated magnetic profiles in (LaMnO$_3$)$_{2n}$/SrMnO$_3$ superlattices$^1$. S.J. MAY, S.G.E. TE VELTHUIS, MSD, Argonne National Laboratory, M.R. FITZSIMMONS, Los Alamos National Laboratory, A.B. SHAH, J.M. ZUO, X. ZHAI, J.N. ECKSTEIN, University of Illinois, Urbana-Champaign, S.D. BADER, A. BHATTACHARYA, MSD and CNM, Argonne National Laboratory — We have determined the magnetic depth profile of MBE-grown ferromagnetic (LaMnO$_3$)$_{2n}$/SrMnO$_3$ superlattices, where $n$ is nominally equal to 3 and 5. Polarized neutron reflectivity measurements reveal the existence of a modulated magnetic structure that repeats with the superperiod in both samples. For $n=5$, a moment of $\sim -2.6 \mu_B$/Mn is measured in the LaMnO$_3$ (LMO) layer, while the moment in the middle of the SrMnO$_3$ (SMO) layer is negligible. The magnetization at the interfaces is found to be asymmetric with an enhanced moment residing at the LMO/SMO interfaces but not at the SMO/LMO interfaces. The origin of the magnetic asymmetry at the interfaces is elucidated from comparison with the structural properties determined by x-ray reflectivity and transmission electron microscopy.

$^1$Supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

10:00AM A31.00009 Complex oxide F/S/F trilayers. C. VISANI, Z. SEFRIOU, C. LEON, J. SANTAMARIA, Universidad Complutense de Madrid, Spain, S.G.E. TE VELTHUIS, A. HOFFMANN, Argonne National Laboratory, NORBERT M. NEMES, M. GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid, Spain, M.R. FITZSIMMONS, B.J. KIRBY, Los Alamos National Laboratory — The origin of the large magnetoresistance in epitaxial F/S/F trilayers composed of highly spin polarized ferromagnetic La$_{1-x}$Ca$_x$MnO$_3$ and high-$T_c$ superconducting YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) is investigated by characterizing the magnetic structure. Polarized neutron reflectometry experiments have determined the detailed magnetization profiles in trilayers with varying YBCO layer thicknesses. In addition to inhomogeneous magnetization profiles, rotation of the magnetization during the magnetization reversal for the films with thick ($\geq 17.7$ nm) YBCO layers has been observed. The results are consistent with the presence of an (in plane) easy-axis tilted away from the (100) direction.

10:12AM A31.00010 Origins of Anomalous Ferromagnetism in F/AF LCMO Multilayers. B. J. KIRBY, S. M. WATSON, National Institute of Standards and Technology, M. KAREEV, J. CHAKHALIAN, University of Arkansas — Unexpected behavior can emerge from magneto-electronic interactions at the interface between two different strongly correlated electron systems. Exchange bias - giving a ferromagnet (F) a preferred direction via coupling with an antiferromagnet (AF) - is a phenomenon of great fundamental and applied research interest. Both topics are pertinent in the case of the interface between F and AF La$_1-x$Ca$_x$MnO$_3$ (LCMO) layers. Depending on $x$, LCMO can be F ($x = 1/3$ Ca) or AF ($x = 2/3$ Ca), and exchange bias has been reported in superlattices consisting of such layers. Surprisingly SQUID magnetometry has shown that the saturation moment of such a structure increases as the nominally AF layer thickness is increased [1]. This has been attributed to electronic effects that cause F order to extend into the nominally AF layer. However, the location of the extra moment cannot be determined with bulk magnetometry techniques. Thus, we have used polarized neutron and x-ray reflectometry to measure the magnetic and structural depth profiles in an exchange biased $x=1/3$ LCMO / $x=2/3$ LCMO bilayer. Our results suggest that the magnetic profile extends beyond the $x = 1/3$ layer, implying that some F order indeed exists in the nominally AF $x = 2/3$ layer. [1] G. Campillo, et al., J. Appl. Phys. 97, 10K104 (2005).

10:24AM A31.00011 Ferroelectric field effect modulation of the magnetic properties of colossal magnetoresistive La$_{1-x}$Sr$_x$MnO$_3$. JASON HOFFMAN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University, HAIJUO MOLEGRAAF, DPMC, University of Geneva, CHANG HONG, Department of Materials, Pennsylvania State University, JEAN-MARC TRISCONE, DPMC, University of Geneva, C.H. AHN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University — In this work, we have tuned the magnetic properties of the colossal magnetoresistive oxide La$_{1-x}$Sr$_x$MnO$_3$ (LSMO) using a ferroelectric field effect approach. Epitaxial LSMO thin films and ferroelectric Pb(Zr,Ti)O$_3$ (PZT) / LSMO heterostructures were fabricated using off-axis RF magnetron sputtering. LSMO films with high crystalline quality and atomically smooth surfaces have been achieved. Using the magneto-optical Kerr effect (MOKE), we measured a shift in the Curie temperature ($T_c$) of LSMO upon switching the polarization direction of PZT, in agreement with the modulation of $T_c$ found from magnetotransport measurements. Unlike the traditional chemical doping approach, the ferroelectric field effect approach allows one to control the magnetism in the system reversibly, without introducing additional lattice disorder/distortion.

10:36AM A31.00012 Structure and properties of CaMnO$_3$/SrMnO$_3$/BaMnO$_3$ superlattices from first principles. SHEN LI, SEONGSHIK OH, KARIN RABE, Department of Physics and Astronomy, Rutgers the State University of New Jersey, Piscataway, 08854, USA — Previous theoretical and experimental studies have shown that three-component, or “tri-color” superlattices can exhibit intrinsic electric polarization due to inversion-symmetry breaking in the layer sequence. In ferromagnetic inversion-symmetry-breaking superlattices, controlled rotation of the magnetization during the magnetization reversal for the films with thick ($\geq 17.7$ nm) YBCO layers has been observed. The results are consistent with the presence of an (in plane) easy-axis tilted away from the (100) direction.

10:48AM A31.00013 Phase separation at the La$_{1-x}$Sr$_x$CoO$_3$ / SrTiO$_3$ (001) interface from thickness and doping dependent magnetotransport$^1$. M.A. TORIJA, M. SHARMA, C. LEIGHTON, University of Minnesota — Bulk La$_{1-x}$Sr$_x$CoO$_3$ (LSCO) has received considerable attention with regard to nanoscale magnetic phase separation. Fabrication of epitaxial films provides a means to study this phase separation under dimensional confinement and at interfaces. Moreover, the characteristic intercluster “GMR” effect observed in the phase-separated state of this material provides a simple means to probe phase separation even in very thin films. We have found that even at $x = 0.5$ (a homogeneous ferromagnetic metal in bulk), sufficiently thin films ($< 60$ Å) grown on SrTiO$_3$ (001) show a crossover to a reduced moment insulating phase, with the characteristic intercluster MR effect. i.e. phase separation occurs. By measuring the thickness dependence of the magnetotransport as a function of doping we have assembled a three-dimensional phase diagram in temperature-doping-thickness space. The interfacial phase-separated region increases dramatically as $x$ is decreased (to over 250 Å at $x = 0.2$) and the non-ferromagnetic phase boundary is approached. The increased prominence of phase separation as proximity to the non-ferromagnetic phase is increased provides a strong hint to the origin of this interfacial phase separation.

$^1$Work supported by NSF DMR.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A32 GMAG: Disordered Magnetic Materials Morial Convention Center 225
8:00AM A32.00001 Transport in strongly disordered classical spin chains, VADIM OGANESYAN, Yale University, ARUJET PAL, DAVID HUSE, Princeton University — We present a numerical study of diffusion of energy at high temperature through strongly disordered arrays of interacting classical spins with Hamiltonian dynamics. We find that quenched randomness strongly supresses transport, with diffusion constant apparently becoming smaller than any power of spin-spin interaction rescaled by randomness. We have looked for but not found signs of a classical many-body localization transition at any finite strength of disorder.

8:12AM A32.00002 Ferromagnetism in Melt-spun Gd\textsubscript{0.946}Fe\textsubscript{0.054}, PAUL SHAND, NICHOLAS JENSEN, JUSTIN BOHNET, University of Northern Iowa, JARED GÖERTZEN, JEFFREY SHIELD, University of Nebraska-Lincoln, DAVID SCHMITTER, Providence College, GEOFFREY SHELBURNE, DIANDRA LESLIE-PELECKY, University of Nebraska-Lincoln — The ac susceptibility and dc magnetization at various temperatures were measured for a melt-spin Gd\textsubscript{0.946}Fe\textsubscript{0.054} alloy. The grain size was \( \approx 100 \) nm. A sharp paramagnetic-to-ferromagnetic transition was observed at a temperature close to that of pure Gd. Effective exponents of the critical temperature and the critical temperature \( T_C \) were extracted by using modified Arrrott plots and Kouvel-Fisher analysis. The values obtained were \( \beta_{eff} = 0.398 \pm 0.004 \), \( \gamma_{eff} = 1.24 \pm 0.02 \), \( \delta_{eff} = 3.83 \pm 0.05 \), and \( T_C = 290.25 \pm 0.17 \) K. These exponent values do not satisfy the Widom scaling relation \( \delta = (3-\gamma_{eff})/\beta_{eff} \). The \( \beta_{eff} \) and \( \gamma_{eff} \) values for ms-Gd\textsubscript{0.946}Fe\textsubscript{0.054} are similar to those obtained for pure Gd in the same temperature interval around \( T_C \). This is in consonance with x-ray microanalysis measurements indicating that the grains are nearly pure Gd. The lower-than-expected value of \( \delta_{eff} \) may be due to the effect of increased anisotropy due to the presence of Fe in the grain-boundary regions.

8:24AM A32.00003 Observation of spin-wave mediated Altshuler-Aronov and weak localization corrections to the conductivity in thin films of gadolinium, RAJIV MISRA, ARTHUR F. HEBARD, KHANDKER MUTTALIB, University of Florida, Gainesville, FL, USA, PETER WOELFLE, IJKM, Universität Karlsruhe, Germany — We present a study of quantum corrections to the conductivity tensor of thin ferromagnetic gadolinium films. Using the sheet resistance as a measure of disorder, in situ magnetotransport studies were performed on a series of gadolinium films deposited onto sapphire substrates having sheet resistance \( R_0 = R_{xx} (5K) \) varying over the range 428 \( \Omega \) (\( \approx 135\)Å) to 4011 \( \Omega \) (\( \approx 35 \) Å). For temperatures \( T < 30 \) K and \( R_0 < 4011 \) \( \Omega \), we observe the simultaneous presence of two types of quantum correction to the Drude conductivity, \( \sigma = \sigma_{Drude} + \Delta \sigma_{SpinWaveMediated} + \Delta \sigma_{WL} \). The characteristic feature of the first correction is an approximately linear increase with temperature of conductivity, and we attribute this as a spin-wave mediated Altshuler-Aronov correction to conductivity. The second correction to the Drude conductivity comes from weak localization, with a characteristic logarithmic temperature dependence of conductivity with a prefactor \( e^2/2\pi^2 h \) in 2D. We observe a breakdown of this behavior at a sheet resistance \( R_0 = 4011 \Omega \), which is very close to the quantum of resistance, \( h/e^2 \approx 41000 \).

8:36AM A32.00004 Monte Carlo study of the three-dimensional Coulomb glass, BRIGITTE SURER, HELMUT G. KATZGRABER, Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland, GERGELY T. ZIMANYI, Department of Physics, University of California, Davis, California 95616, USA, BRANDON A. ALLGOOD, Numerate Inc., 1150 Bayhill Drive, San Bruno, CA 94066, USA — The memory and hysteretic effects found in strongly-disordered electron systems can be explained by the existence of a glassy phase, the Coulomb glass. Efros and Shklovskii have predicted the emergence of a soft Coulomb gap, resulting from the long-range interactions between the localized electrons. However, the relationship between the soft Coulomb gap in the density of states and the electron's glassy behavior has been a long-standing unresolved question. Only recently has it been surmised within the framework of a mean field theory that the disordered electron system undergoes a replica symmetry breaking transition at a finite temperature, similar to the Sherrington-Kirkpatrick model of spin glasses. Because it is not clear, however, whether the transition persists beyond the mean-field approximation, we study in detail the critical behavior and the shape of the Coulomb glass in three space dimensions using Monte Carlo methods. Furthermore, we compare our results for the (random-energy) Coulomb glass model to previous results on a random lattice version of the model. Since these models possess different symmetries, the equivalence of the phase diagrams is far from obvious, contrary to previous claims.

8:48AM A32.00005 Reentrant spin-glass behavior and enhanced Curie temperature in epitaxial MnSi, ERIC KARHU, SAMER KAHWAJI, TED MONCHESKY, Dalhousie University, KRISTA RAFFEL, MICHAEL ROBERTSON, Acadia University, CHRISTIAN MAUNDERS, McQuaid-Stewart, Buchan, Canada — We grew single crystal MnSi(111) thin films on Si(111) substrates by molecular beam epitaxy. The 3\% lattice mismatch created an in-plane tensile strain of \( \epsilon_l = 0.005 \pm 0.001 \), as measured by transmission electron microscopy, and induced an out-of-plane compressive strain \( \epsilon_z = -0.0033 \pm 0.0001 \), as determined by x-ray diffraction. The MnSi(111) films displayed two magnetic phases. The first transition from a paramagnetic phase to a phase with long range magnetic order occurs with an enhanced Curie temperature \( T_C = 40 \) K as compared to bulk MnSi, which develops helical magnetic structure below \( T_C = 29.5 \) K. This increase in \( T_C \) can be explained by an in-plane strain. A second phase transition to spin glass, below \( T_f = 35 \) K, maybe due to geometric frustration created by the compressive out-of-plane strain. We propose a relationship between the reentrant spin-glass behavior and the partial magnetic order reported for bulk MnSi under pressure.

The authors gratefully acknowledge the support received from NSERC and Dr. G. Bolton and the Canadian Centre for Electron Microscopy.

9:00AM A32.00006 Dynamical behavior of spin clusters in La\textsubscript{1-x}Sr\textsubscript{x}CoO\textsubscript{3}, ROBERT SMITH, MICHAEL HOCH, WILLIAM MOULTON, PHILLIP KUHNS, GREGORY BOEBINGER, ARNEIL REYES, National High Magnetic Field Lab, JOHN MITCHELL, Argonne National Lab — Previous work has provided evidence for magnetic glassing behavior in the hole-doped cobaltite system La\textsubscript{1-x}Sr\textsubscript{x}CoO\textsubscript{3}(LSCO). Models proposed to describe the interesting and unusual magneto-transport properties of LSCO involve hole-rich clusters in a hole-poor matrix. The glassy properties, which are not well understood, have variously been interpreted in terms of spin glass and cluster glass components. The present 1\textsuperscript{39}La NMR spectral line shapes on single crystal LSCO, that map the hyperfine field distribution in the \( x-T \) plane, confirm the presence of magnetic clusters, identified as spin polaron, and provide a phase inhomogeneity diagram. NMR relaxation rates have been used to probe the dynamical behavior of the system at the nanoscale level in macroscopically insulating and metallic samples as a function of temperature in the range 4-280 K. For \( x \) less than the metal-insulator critical concentration \( x_{C} = 0.17 \) value has been obtained for two classes of glassy component with different characteristic correlation time distributions and freezing temperatures. The magnetic glass properties persist above \( x_{C} \). A spin polaron model is used to explain the results.

9:12AM A32.00007 Local field distributions in spin glasses, DAVID SHERRINGTON, University of Oxford, HELMUT G. KATZGRABER, ETH Zurich, STEFAN BOETTCHER, Emory University — Numerical results for the local field distributions of a family of Ising spin-glass models are presented. In particular, the Edwards-Anderson model in dimensions two, three, and four is considered, as well as spin glasses with long-range power-law-modulated interactions that interpolate between a nearest-neighbor Edwards-Anderson system in one dimension and the infinite-range Sherrington-Kirkpatrick model. Remarkably, the local field distributions only depend weakly on the range of the interactions and the dimensionality and show strong similarities except for near zero local field.

9:24AM A32.00008 ABSTRACT WITHDRAWN —
9:36AM A32.00009 The Antiferromagnetic SO(3) Heisenberg Quantum Spin-Glass with Short Range Interaction, EDUARDO MARINO, Princeton University, CARLOS CONCEICAO, UFRJ — We study the quenched disordered magnetic system which is obtained from the 2D SO(3) Heisenberg model, with nearest neighbors interaction, by taking the random values of the exchange couplings as given by a Gaussian probability distribution centered in a value of the coupling that corresponds to anti-ferromagnetic order. Using coherent states, we map this system onto a generalization of the SO(3) nonlinear sigma model, containing different flavors, which correspond to the replicas and a quartic interaction. We then integrate over the transverse components and perform a mean-field calculation of the free energy density in the limit of zero replicas. The phase diagram of the system is then obtained and shows a critical curve, starting at a quantum critical point at $T=0$ separating a paramagnetic from a spin-glass phase. The stability of the phases is demonstrated by an analysis of the Hessian matrix of the free energy.

9:48AM A32.00010 On the ordering of Ising spin glasses in a field, HELMUT G. KATZGRABER, Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland, THOMAS JÖRG, LPTMS, UMR 8626 CNRS et Univ. Paris-Sud, 91405 Orsay CEDEX, France, FLORENT KRZAKALA, Laboratoire PCT, UMR Gulliver CNRS-ESPCI 7083, 10 rue Vauquelin, 75231 Paris CED — We study the existence of a spin-glass phase in a magnetic field in three space dimensions using a novel approach where the Monte Carlo simulations are performed along a nontrivial path in the magnetic field–temperature plane which must cross any putative de Almeida-Thouless line. The method is first tested on the mean-field version of the Edwards-Anderson Ising spin glass on a Bethe lattice where we compute analytically the instability line that separates the spin glass from the paramagnetic state. While the de Almeida-Thouless line is clearly reproduced by our simulations on the mean-field Bethe lattice, no such instability line can be found numerically for the short-range three-dimensional model. We thus conclude that there is no such instability line for three-dimensional short-range Ising spin glasses.

10:00AM A32.00011 Spin glass of a diluted Ising dipolar system, KA-MING TAM, MICHEL GINGRAS, University of Waterloo — The diluted dipolar Ising system has been regarded as a standard example which exhibits spin glass properties. Recent studies have challenged the existence of spin glass phase transition in one of the materials in this category, $\text{LiHo}_x\text{Y}_{1-x}F_4$. Using Monte Carlo simulations, we calculate various quantities to address the current controversy of a possible spin glass phase transition in this material. Beside the conventional method to locate the spin glass transition by observing the crossing of Binder ratios of magnetization moments, another crucial probe for the nature of spin glass, order parameter fluctuations, is studied via the so-called fluctuation sensitive parameters. Crossing is observed in the Binder ratio of overlap order parameter, and non-trivial structures of overlap order parameter are obtained at low temperature.

10:12AM A32.00012 Nonlinear and ac Susceptibility of the Dilute Ising Magnet $\text{LiHo}_x\text{Y}_{1-x}F_4$, JEFFREY QUILLIAM, SHUCHAO MENG, CHAS MUGFORD, JAN KYCIA, Department of Physics and Astronomy, University of Waterloo — Recent work has called into question the existence of a spin glass phase transition in the dilute dipolar Ising magnet $\text{LiHo}_x\text{Y}_{1-x}F_4$. Other work has suggested that there is an exotic spin liquid phase found at a Ho concentration of $x = 0.045$ [2]. In order to carefully study the dynamics of this system, we have put together a SQUID magnetometer which allows for measurements of ac susceptibility and nonlinear susceptibility over a large frequency range. We present results from measurements on single crystals of $\text{LiHo}_x\text{Y}_{1-x}F_4$, particularly on an $x = 0.045$ sample, in an attempt to either reproduce the exotic “anti-glass” physics that was previously observed or to detect a spin glass transition. [1] P. E. Jonnson et al. PRL 98, 256403 (2007) [2] S. Ghosh et al. Science 296, 2195 (2002)

1 Funding provided by NSERC, CFI, OIT, MNO and The Research Corporation

10:24AM A32.00013 Low-temperature properties of the dilute dipolar magnet $\text{LiHo}_x\text{Y}_{1-x}F_4$, ANDERS BILTMO, PATRIK HENELIUS, KTH, Stockholm — The phase diagram of the rare-earth compound $\text{LiHo}_x\text{Y}_{1-x}F_4$ is considered as a function of dilution as given by a Gaussian probability distribution centered in a value of the coupling that corresponds to anti-ferromagnetic order. Using coherent states, the ground state of the system is ferromagnetic and as $x$ decreases a disordered ground state with glassy properties arises. If $x$ is decreased further, the system enters a phase sometimes referred to as “antiglass”. Both the non-canonical glassy state and the not yet understood “antiglass”, have never been systematically studied using a microscopic probe. We performed muon spin relaxation measurements in five samples ($x=0.018$, 0.045, 0.08, 0.12 and 0.25) which span these disordered phases. In this talk we will show from the microscopic point of view, how does the glassy state manifests itself as well as how does the evolution from the glass to the “antiglass” occurs.

Monday, March 10, 2008 8:00AM - 10:36AM — Session A33 DMP GMAG FIAP: Focus Session: Spin Dependent Phenomena in Semiconductors: — Morial Convention Center 224
8:00AM A33.00001 Cross-sectional scanning tunneling microscopy of Ga_{1-x}Mn_xAs/GaAs Heterostructures

PEDRAM ROUSHAN, ANTHONY RICHARDELLA, Department of Physics, Princeton University, SHAWN MACK, DAVID AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, ALI YAZDANI, Department of Physics, Princeton University — We have used a cryogenic scanning tunneling microscope (STM) to perform cross-sectional imaging studies of GaMnAs heterostructures. The heterostructures, consisting of a p-type buffer followed by a 3% Mn doped layer, were grown on a n-type GaAs substrate by molecular-beam epitaxy and cleaved in situ for STM measurements. The topographic measurements on the GaMnAs layer showed a variety of long range electronic structure modulations on the order of a few nm due to high level of disorder and compensation. Combining bias-dependent imaging and spectroscopy, we have used the STM to identify electronic features due to Mn dopants and other defects. In particular, we find that Mn dopants on the top most layer act as deep acceptors and exhibit both topographic and spectroscopic features as our previous work [1] on Mn adatoms substituted into GaAs using STM manipulation techniques. [1] D. Kitchen, A. Richarrella, J-M. Tang, M. Flate, A. Yazdani, Nature 442, 436–439 (2006)

1This work is supported by ARO, ONR, NSF and ASEE.

8:12AM A33.00002 Spectroscopic Mapping of Electronic States near Fermi Energy in GaMnAs

ANTHONY RICHARDELLA, PEDRAM ROUSHAN, Department of Physics, Princeton University, SHAWN MACK, DAVID AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, ALI YAZDANI, Department of Physics, Princeton University — We have used atomic resolved spectroscopic mapping with the scanning tunneling microscope (STM) to probe the spatial structure of electronic states in GaMnAs/GaAs heterostructures. Mapping the electronic states over a wide range of energies across the heterostructure, we find significant differences from the p-type buffer layer to the Mn-doped layer. The features include gap narrowing and in gap resonances, some of which are due to the bulk electronic structure of GaMnAs. We focus on these bulk states, in particular a broad state that is observed near the valance band above the Fermi energy. We analyze the spatial distribution of these states in conjunction with our observations of disorder in the sample and variations in the electrostatic potential landscape due to compensation. Finally, we discuss the implications of our results to the questions of localization, band tails and whether highly doped GaMnAs has an impurity band separated from or merged with the host valance band.

This work was supported by ARO and ONR, NSF and ASEE.

8:24AM A33.00003 STM studies of spin-spin interactions between Mn acceptors in p-type GaAs

DONGHUN LEE, DAVID R. DAUGHTON, JAY A. GUPTA, The Ohio State University, Department of Physics — We use a custom STM operating in a cryogenic, ultrahigh vacuum environment to study spin-spin interactions in semiconductors at the single-impurity level. By applying a voltage pulse with the STM tip, single magnetic impurities (e.g. Mn) can be substituted for Ga atoms in the first layer of the GaAs(110) surface. It was previously found that pairs of Mn acceptors exhibit an exchange splitting which depends on their separation and crystal orientation [2]. We are developing a capability for spin-polarized STM to better study long range magnetic ordering between pairs and larger clusters of Mn acceptors. To characterize the magnetic orientation of our STM tips, we have prepared samples such as Co/Cu(111) which exhibits out-of-plane magnetization, and Cr(001), which is an antiferromagnet with in-plane magnetic contrast between alternating terraces. http://www.physics.ohio-state.edu/~jugupta [2] D. Kitchen et al., Nature 442, 436-439 (2006)

Supported by the Beckman Foundation.

8:36AM A33.00004 Magnetic Memory Effects in Coherent Magnetization Dynamics of GaMnAs: From Non-equilibrium to Thermal Regime

INGRID COTOROS, University of California at Berkeley, California, JIGANG WANG, Lawrence Berkeley National Laboratory, California, XINYU LIU, JACEK FURDYNA, University of Notre Dame, Indiana, JAROSLAV CHOVAN, ILIAS PERAKIS, University of Crete, Heraklion, Greece, DANIEL CHEMLA, University of California at Berkeley, California — III-Mn-V heterostructures exhibit rich spin memory effects and their magnetic properties show strong responses to external stimuli (light, electrical gate and current) via carrier density tuning. Here we report on the coherent magnetization dynamics due to laser excitation of transient carriers in GaMnAs, distinctly depending on the initial magnetic state the system is prepared in. We identify two distinct temporal regimes that reveal a complex scenario of spin reorientation, marked by the transition from a highly non-equilibrium, non-thermal, transient carrier-mediated regime (< 300 femtosecond), to a thermal, lattice-heating regime (on the picosecond time scale). The ultrafast, sub-picosecond response can be used as footing for ultrafast optical detection of magnetic memory states. This observed femtosecond cooperative magnetic phenomenon may represent an as-yet-undiscovered universal principle in all carrier-mediated ferromagnetic materials, offering potential perspectives for terahertz (10^{12} Hz) speed “spintronic” devices and functional systems.

8:48AM A33.00005 Epitaxial engineering of ferromagnetism in (GaAs)/(Ga,Mn)As digital superlattices

M.J. WILSON, G. XIANG, B.L. SHEU, P. SCHIFFER, N. SAMARTH, Penn State University — Recent theory predicts novel pathways for the epitaxial engineering of ferromagnetism in GaAs/MnAs digital superlattices grown along different crystalline directions [Francosetti et al., PRL 97, 047202 (2006)]. This has motivated us to systematically study GaAs/(Ga,Mn)As digital superlattices grown along the [001], [110], [210] and [311] directions. We have characterized these samples using SQUID magnetometry, magnetotransport, TEM and SIMS. We observe clear trends in the Curie temperature that are correlated with the epitaxy direction and the GaAs spacer layer thickness. Our results suggest that – for a given Mn concentration – the Curie temperature of (Ga,Mn)As may depend on the geometrical arrangement of the Mn ions. We also explore alternative explanations, such as an orientation dependence of the Mn incorporation rate and defect formation energies.

Work supported by the DARPA PROM program

9:00AM A33.00006 Stoichiometric growth of high Curie temperature heavily-alloyed GaMnAs

S. MACK, R.C. MYERS, J.T. HERON, A.C. GOSSARD, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Previous work indicates that single-phase, high-Mn incorporation (>9%) in GaAs can be obtained via MBE at very low substrate temperatures with film thicknesses on the order of a few nanometers. Here we present the properties of smooth, single-crystalline GaMnAs samples with Mn densities between 9 and 18% and continuously tuned arsenic stoichiometry using a combinatorial, non-rotated growth method. [1] Systematic, reproducible thick films (100 nm) display optimal magnetic, electronic, and structural properties in a narrow band of As:Ga flux ratios at the stoichiometric condition, where the Curie temperature is maximum. Post-growth annealing increases the Curie temperature while lowering the lattice constant, indicating that Mn interstitials are the dominant compensating defect in high-Mn containing GaMnAs. Curie temperatures from many samples grown with varying conditions all reach a maximum near the previously reported maximum (~165K).


Work supported by ONR, AFOSR, and the ASEE.

\textsuperscript{1}This research is supported by NSERC, CFI, and the Canada Research Chairs program.

9:24AM A33.00008 Magnetic domain structure study of a ferromagnetic semiconductor using a home-made low temperature scanning Hall probe microscope\textsuperscript{1}, SEONGSOO KWEEON, Materials Science and Engineering, ALEX DE LOZANNE, Department of Physics, U Texas at Austin, NITIN SAMARTH, Physics Department, Penn State U,University Park, PA — GaMnAs is a ferromagnetic semiconductor actively studied for basic research and for the possibility of application to spintronic devices. To study the local magnetic properties of this material the magnetic force microscope (MFM) is too invasive (by affecting the domains in the sample) or not sensitive enough (due to the weak magnetization of the GaMnAs). We have therefore developed a scanning Hall probe microscope (SHPM) to complement our MFM studies. We use a lock-in technique to supply a bias current of 1-10\textmu A and to measure the Hall voltage. We have used this home-made SHPM in conjunction with a computer hard disk sample. Comparing images of this sample obtained with MFM and SHPM we show that our home-made SHPM is operating well. We observed the domain structure of 30-nm thick Ga\textsubscript{0.99}Mn\textsubscript{0.01}As epilayer grown on a 700nm-thick In\textsubscript{0.13}Ga\textsubscript{0.87}As buffer covering a GaAs substrate. We will study the magnetic domain structure as a function of temperature with varying external magnetic fields.

\textsuperscript{1}Supported by NSF DMR-0308575

9:36AM A33.00009 Si co-doping of GaMnAs: a solution for removing As antisites , Y.J. CHO, X. LIU, J.K. FURDYNA, University of Notre Dame — The primary defects that degrade the ferromagnetism of GaMnAs are believed to be Mn interstitials and As antisites. The former can be reduced by low temperature annealing after growth. However, so far no solution for removing As antisites in GaMnAs has been developed. In this connection we report the effect of Si co-doping on Ga\textsubscript{1-x}Mn\textsubscript{x}As films. For x < 0.05, Si co-doping decreases the Curie temperature compared to undoped GaMnAs. However, at higher Mn concentration Si co-doping has the desirable effect of improving both ferromagnetic and structural properties of GaMnAs. To achieve a high Mn concentration in GaMnAs the growth temperature has to be sufficiently low to prevent the formation of MnAs clusters, but this introduces a high density of As antisites in GaMnAs, thus degrading its structural and ferromagnetic properties. However, when such growth of GaMnAs is accompanied by Si co-doping, x-ray diffraction results show that such co-doping removes almost all As antisites in GaMnAs with high Mn concentration. Furthermore, magneto-transport and magnetization measurements show that the ferromagnetic properties of thick Si co-doped Ga\textsubscript{1-x}Mn\textsubscript{x}As (x > 0.1) films are greatly improved compared to samples without Si. This suggests that Si co-doping provides an effective solution for removing As antisites in GaMnAs at high Mn concentrations.

9:48AM A33.00010 Ferromagnetism in epitaxial InMnSb films , NIDHI PARASHAR, BRUCE WESSELS, Northwestern University — The structure and ferromagnetic properties of epitaxial In\textsubscript{1-x}Mn\textsubscript{x}Sb semiconductor films deposited using metal-organic vapor phase epitaxy were investigated. Films were single phase as determined by x-ray diffraction for x = 0.01 to 0.05. A rocking curve width of 0.3 degrees was measured in 2\textTheta-x-ray scans. XRD data is consistent with the formation of self-assembled Mn-rich nanocolumns. These nanocolumns are observed in a wide range of growth temperatures (80°C to 180°C) and Mn concentrations (1% to 11%). However the deposition rate is kept very low in order to favor the 2D spinodal decomposition which promotes the growth of nanocolumns. In this talk, we first present a complete phase diagram of nanocolumns as a function of growth temperature and Mn concentration focusing on their size, density, crystalline structure and magnetic properties. In particular, we could demonstrate that at low growth temperature it is possible to tune the columns density and at higher growth temperatures their size distribution. Moreover vertical self-organization of nanocolumns in (GeMn/Ge) superlattices could be achieved. At low growth temperatures, nanocolumns exhibit the diamond structure of Ge and contain up to 30 % of Mn. By combining ab-initio calculations and EXAFS measurements, we could suggest a realistic building block of the nanocolumns. In parallel we have studied the crystalline structure of nanocolumns using grazing incidence x-ray diffraction on synchrotron radiation facilities. We then correlated the magnetic properties like magnetic anisotropy of nanocolumns to their structure by combining SQUID and EPR measurements in a three-dimensional geometry. Finally magneto-transport measurements were performed to evidence the coupling between carriers and the magnetic nanocolumns. CIP measurements mostly give information on the Ge matrix electronic properties and CPP measurements on the nanocolumns. We show the first CPP measurements on a single nanocolumn using nanointerfaces.

Monday, March 10, 2008 8:00AM - 10:48AM — Session A35 FIAP: Focus Session: Negative Index Materials I Morial Convention Center 227

8:00AM A35.00001 Discrete Breathers in magnetic metamaterials in one and two dimensions, GIORGOS TSIRONIS, MARIA ELEFTHERIOU, NIKOS LAZARIDES, Physics Department, University of Crete, and IESL, Foundation of Research and Technology, P. O. Box 2208, 71003, Heraklion, Greece — We study the formation, stability as well as mobility of discrete breathers (DBs) in magnetic metamaterials in one and two dimensions. Magnetic metamaterials consists of split ring resonators (SRRs) exhibit large magnetic response at Terahertz and optical frequencies. We use nonlinear arrays of SRRs where DBs arise as a result of the nonlinearity and discreteness. We consider different geometries of SRRs in both dimensions and find several different types of Hamiltonian nonlinear excitations such as dark, single-site and multibreathers. We also consider the dissipative version of the problem where DBs are formed as well. In the latter case, DBs locally alter the paramagnetic character of MMs to a diamagnetic.
8:12AM A35.00002 Negative response and intrinsic localization in rf SQUID metamaterials.

GEORGE TSIRONIS, NIKOLAOS LAZARIDES, MARIA ELEFFTERIOU, University of Crete, and Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas — A periodic array of rf SQUIDs in an alternating magnetic field acts as an inherently nonlinear magnetic metamaterial, due to the nonlinearity of the Josephson element and the resonant properties of the SQUIDs themselves. Neighboring SQUIDs are weakly coupled due to magnetic dipole-dipole interaction through their mutual inductances, allowing an effective medium description if the wavelength of the applied field is much larger than the array period. We found that SQUID arrays can provide negative magnetic response, and thus negative permeability, above the resonance frequency of the individual SQUIDs. Moreover, that response can be tuned by the applied flux. Dissipative SQUID arrays, modeled as discrete networks, support nonlinear excitations in the form of intrinsic localized modes (discrete breathers). We found that dissipative discrete breathers exist in both one- and two-dimensional SQUID arrays. Furthermore, those breathers alter locally the magnetic response of an array from paramagnetic to diamagnetic or vice versa.

8:24AM A35.00003 Hybrid metamaterials for dynamic tuning

TOM DRISCOll, University of California San Diego, SABARNI PALIT, Duke University, MUMTAZ QAZILBASH, University of California San Diego, MARCUS BREHM, F. KEILMANN, Max-Planck-Institut, B. CHAE, H. KIM, IT Convergence & Components Lab, DIMITRI BASOV, University of California San Diego, NAN MARIE-JOKERST, DAVID SMITH, Duke University — Advances in the field of metamaterials have created many new and exciting devices, but the performance and applicability of these devices to date have been hindered by the reliance on a dispersive resonance. In this talk we present a metamaterial device with the ability to dynamically tune the center frequency of its far-infrared resonance in real-time, alleviating many of the limitations of dispersion. Our device combines the familiar Split Ring Resonator (SRR) element with a thin film of rare earth oxide possessing a metal-to-insulator phase transition that occurs just above room temperature. During this phase transition, the electromagnetic responses of the oxide-film and SRR become intertwined, creating a sort of hybrid metamaterial. This interaction allows us to manipulate the resonance of the SRR via the oxide-film material properties. The device exhibits a dynamically tunable resonance — shifting center frequency of the magnetically active SRR mode by as much as 20% within 2 degrees Kelvin of temperature control.

8:36AM A35.00004 Tunable plasmonic nanostructures and nanolenses in optical domain

A.M. BRATKOVSKY, Hewlett-Packard Laboratories — We have designed and studied various periodic metamaterials with the resonant response in the IR and optical range. In particular, the stacks of metallic films with periodic hole arrays separated by dielectric layers (fishnet, FN) have been demonstrated to have a negative index at IR frequencies. We were able to control the index of refraction of a fishnet with an amorphous semiconductor spacer layer in a pump-probe experiment [1]. This opens up ways for modulating the light at the nanoscale. We have also observed strong second- and third- harmonic generation with this metamaterial. We discuss various uses of a gain material to compensate the losses. Arrays of metallic nanoparticles or holes support individual and collective plasmonic excitations that contribute to surface enhanced Raman scattering (SERS) with thousand-fold field enhancement factor that can be used for single-molecule detection and other applications of the “light at the nanoscale.”

1 In collaboration with E.V. Ponizovskaya, E. Kim, Wei Wu, Z. Yu, S-Y Wang, Y.R. Shen, R.S. Williams

9:12AM A35.00005 Negative Refraction Index in Magnetic Semiconductors

ADIL-GERAI KUSSOW, University of Massachusetts Lowell, Department of Physics, ALKIM AKYURTLU, University of Massachusetts Lowell, Electrical and Computer Engineering Department — A novel principally homogeneous, non-composite magnetic semiconductor, or Chromium doped Indium Oxide, with the Curie temperature well above room temperature with natural negative refraction index in the THz range will be presented. The negative refraction index arises due to the overlapping of the negative permittivity in the plasmon subsystem and the negative permeability in the spin wave (magnon) subsystem within the same frequency domain. Since the losses in the magnetic mode are almost negligible, and the additional scattering losses due to the inhomogeneities are not present in our homogeneous medium, the total losses are exclusively due to the plasmon decay. Consequently, the negative refraction index wave has losses approximately 5 times smaller than losses in any of the currently known inhomogeneous designs. The parameters of both plasmon and magnon subsystems are calculated from the extended Band Theory, and first principles, respectively, and validated with available experimental data. Analytical expressions which describe the negative refraction index band are also presented.

9:24AM A35.00006 Negative refraction and an optical analogue of a directional spin valve in multiferroic materials

KEI SAWADA, RIKEN, SHUICHI MURAKAMI, Tokyo Institute of Technology, NAOITO NAGAOSA, CREST, The University of Tokyo — We present a new mechanism for negative refraction caused by a magnetoelectric (ME) effect. The ME effect appears in multiferroic materials in which spatial inversion and time-reversal symmetries are simultaneously broken. Such symmetry breakings allow us to control the spontaneous electric polarization by a magnetic field. We study polaronic states in multiferroics and show that an asymmetric dispersion relation due to the ME effect gives rise to an optical analogue of a directional spin valve and a one-way waveguide as well as the negative refraction. We also estimate a realistic size of the effect.

9:36AM A35.00007 Infrared Properties of NiO-SrTiO3 Composites

I.D. VUGMEYSTER, K. KASTELLA, C. KNILL, R. MERLIN, J.F. WHITAKER, J.A. AZURDIA, S.N. KARLSDOTTIR, V. VOMECKOVA, C. TORRES-GARIBAY, J.W. HALLORAN, U. Michigan, G.O. ANDREEV, D.N. BASOV, U. California San Diego — Magnetic-dielectric composites with overlapping magnetic- and electric-dipole resonances are promising candidates in the search for artificial systems with negative refractive index [1]. Here we report on the fabrication and infrared characterisation of NiO-SrTiO3 ceramics. Transmission and reflection data were obtained in the 10-700 cm−1 range using both a THz time-domain and a FTIR spectrometer. The spectra show features associated with the bulk antiferromagnetic resonance of NiO and the soft mode of SrTiO3, as well as new collective modes of the aggregate. The results are in qualitative agreement with effective medium theories.

1Supported by AFOSR MURI

9:48AM A35.00008 Measurements of the electric susceptibilities of Au nanorods at optical frequencies

JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, NICHOLAS KOTOV, ASHISH AGARWAL, University of Michigan — Accurate knowledge of the electric susceptibilities of nanoparticles is of key importance in the design of optical metamaterials. We have determined the principal values of the susceptibility tensor of Au nanorods by measuring the real and imaginary phase shift of light transmitted by Au nanorod suspensions in organic solvents. The nanorods were aligned by an externally applied low frequency electric field. The real and imaginary parts of the phase shift were determined using a conoscopic Mach-Zehnder interferometer with a dye laser and a spectrophotometer, respectively. We discuss our procedure of extracting the principal values of the susceptibility tensor as function of wavelength from the experimental data. We consider the implications of our results for the construction of optical negative index metamaterials.

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.
10:00AM A35.00009 Tuned permeability in terahertz split-ring resonators for devices and sensors, GREG ANDREEV, TOM DRISCOLL, DIMITRI BASOV, MASSIMILIANO DIVENTRA, University of California at San Diego, SABARNI PALIT, SANG YEON CHO, NAM MARIE JOKERST, DAVID SMITH, Duke University — A process is demonstrated for tuning the magnetic resonance frequency of a fixed split-ring resonator array, by way of adding material near the split-ring elements. Applying drops of a silicon-nanospheres/ethanol solution to the surface of the sample decreases the magnetic resonance frequency of the split-ring array in incremental steps of 0.03 THz. This fine tuning is done post fabrication and is demonstrated to be reversible. The exhibited sensitivity of the split-ring resonance frequency to the presence of silicon nanospheres also suggests further application possibilities as a sensor device.

10:12AM A35.00010 Double Negative Index of Refraction Observed in a Single Layer of Closed Ring Resonators, ZHAO HAO, MICHAEL MARTIN, Advanced Light Source, Lawrence Berkeley National Laboratory, BRUCE HARTENECK, STEFANO CABRINI, Molecular Foundry, Lawrence Berkeley National Laboratory, ERIK ANDERSON, Center of X-Ray Optics, Lawrence Berkeley National Laboratory — We report the results of a spectroscopic study of a single layer of nanoscale metallic single closed ring resonators on a free- standing thin membrane at near-normal and grazing angles of incidence. When the magnetic component of the light is perpendicular to the ring plane, we observe a so-called “double” negative index of refraction at near-infrared frequencies attributed to a strong magnetic dipolar resonance and a broad electric resonance in this metamaterial. We experimentally identify the different resonance modes and the spectral component of the region of negative refractive index on a series of samples with different feature and lattice sizes, using multiplexing and comparing to electromagnetic simulations.


1This work was supported by the LDARD Program and at M. F. by the Office of Science, Office of Basic Energy Sciences, of Lawrence Berkeley National Laboratory under the DOE Contract No. DE-AC02-05CH11231.

10:24AM A35.00011 Z-scan measurement of oriented Au nanoparticle suspensions, PIOTR LESIAK, Warsaw University of Technology, MICHELE MOREIRA, PETER PAlFFY-MUHORAY, Liquid Crystal Institute, KSU, NICKOLAS KOTOV, ASHISH AGARWAL, University of Michigan — The Z-scan technique, developed by the CREOL group, is a simple and effective method for measuring intensity dependent optical nonlinearities of materials. We have carried out Z-scan measurements of gold nanorods suspended in organic solvents using a CW laser. A low frequency external electric field was used to orient the nanoparticles. We present our experimental results for the real and imaginary parts of the nonlinear phase shift as function of the applied aligning electric field. We consider a variety of possible contributing physical mechanisms, and compare their expected contributions with experimental observations. [1] M. Sheik, A.A. Said, and E.W. Van Stryland, Opt. Lett. 14, 955 (1989). [2] J. Fontana, and P. Palffy-Muhoray, APS March meeting 2008, New Orleans, LA (2008).

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

10:36AM A35.00012 Numerical simulation of the non-local optical response of nanoparticles, JEREMY NEAL, PETER PAlFFY-MUHORAY, Liquid Crystal Institute, KSU — The interaction of nanoparticles with light is a primary focus of research in negative index materials. When the wavelength of light is comparable to the particle size, significant non-local effects are expected in the electric and magnetic response of the nanoparticles. It has been suggested that the spatially non-local response may be taken into account via the bianisotropic formalism for the constitutive equations. We have carried out numerical simulations of the optical response of nanoparticles using both the discrete dipole approximation and the finite integration technique to determine the effectiveness of these bianisotropic constitutive equations. We present our results, which indicate that the approach of Agranovich et al.[1] provides a better description of the non-local optical response than the bianisotropic formalism.


1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A36 GIMS: Focus Session: X-ray and Electron Optics and Microscopy Morial Convention Center 228

8:00AM A36.00001 , WENBING YUN, XRadia Corp. — No abstract available.

8:36AM A36.00002 Optimal conditions for combining a transmission x-ray microscope with a grating interferometer, XIANGHUI XIAO, QUN SHEN. Argonne National Laboratory, X-RAY MICROSCOPY & IMAGING GROUP TEAM — Transmission x-ray microscope (TXM) is a powerful imaging tool that can provide resolution down to 15~20 nm. Grating interferometer (GI) is a recently established imaging technique with which both phase and attenuation information of an arbitrary specimen can be extracted in a straightforward way. The achievable resolution of a GI is limited by either the grating analyzer period or the detector pixel size, which is currently at about micron level. It is natural to imagine that combing a TXM with a GI (TXMGI) will give ability to image a weak-absorbing specimen with high resolution. However, it is not trivial to obtain reliable structure information from a TXMGI. In this presentation, we will discuss the dependence of the interferogram on three key parameters in a TXMGI, i.e. the coherence of the illumination beam, the numerical aperture of the TXM, and the grating period. Based on that result, the optimal conditions and the limits on the achievable resolution are obtained.

3Use of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

8:48AM A36.00003 Consideration in the Reconstruction of 3D atomic Structure from X-Ray, YUHAO WANG, NEW JERSEY INSTITUTE OF TECHNOLOGY, J. BAI, UNIVERSITY OF TENNESSEE, T.A. TYSON, NEW JERSEY INSTITUTE OF TECHNOLOGY, P. SIDDONS, G. DE GERONIMO, BROOKHAVEN NATIONAL LABORATORY — X-Ray Holography is a promising technique for recovery of the three dimensional structure of materials. With the advent of high flux sources and fast x-ray detectors this method is under serious consideration as main stream technique. Simulations based on spherical atomic scattering factors method are performed to estimate the effects of wave front curvature by application to specific systems. An assessment is made of the distortions which arise if artifacts such as errors in the position of the origin exists. Simulations are performed to determine the influence of counting rates on the image reconstruction.

3This work is supported by NSF MRI-0722730.
9:00AM A36.00004 Synchrotron topographic studies of stacking faults in type-IIa diamond crystals.  XIANRONG HUANG, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439; Brookhaven National Laboratory, Upton, NY 11973, ALBERT MACRANDEL, JOZEF MAJ, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439 — High-quality diamond is an ideal material for various synchrotron x-ray optical applications. However, diamond crystals generally contain various defects, among which stacking faults (SFs) are more detrimental since they are planar defects extended up to square centimeters. In this presentation, we will introduce monochromatic synchrotron topographic studies of SFs (as well as other defects) in type-IIa diamond crystals. SFs show strong contrast at the tails of the rocking curve, thus broadening the rocking curve width. The outcrops of SFs on the crystal surface still show sharp white-line contrast at the Bragg peak, indicating strong strains or lattice misorientations near the outcrops. From the variation of SF contrast with the rocking angle, we obtain a detailed picture how the extended SFs influence the diffraction performance of diamond crystals. A straightforward diffraction contrast mechanism of SFs will also be presented in addition to the dynamical theory description.

9:12AM A36.00005 Design, nanofabrication and testing of silicon and diamond hard X-ray optics.  A.F. ISAKOVIC, NSLS-Brookhaven National Laboratory, A. STEIN, J.B. WARREN, K. EVANS-LUTTERODT, Brookhaven National Laboratory, S. NARAYANAN, Argonne National Laboratory, M. SPRUNG, A. SANDY, Argonne National Laboratory — We have designed, fabricated and tested silicon (Si) and diamond based X-ray kinoform lenses. In design and nanofabrication of such X-ray optics elements, surface roughness and wall verticality are among the tasks of critical importance for achieving as-designed performance. Our cyclic cryogenic RIE method [1], developed to deal with such stringent nanofabrication requirements, is comparable in performance to licensed Bosch process, as established in measurements of the surface roughness, and the etch rate (>2 microns/min for Si; ~100 nm/min for diamond) and verticality (<1deg over 100 microns) parameters. We compare nanofabrication procedures for Si and diamond lenses, and discuss relative merits of Si and diamond as materials for X-ray lenses. We also show sub-100 nm spot size tests of kinoform Si-based X-ray focusing optics, determined via knife edge measurements at APS 8-ID, and a preliminary results of tests of diamond-based kinoform lens at NSLS, performed at X13B and APS 8-ID. [1] A. F. Isakovic et al., submitted for publication.

9:24AM A36.00006 X-ray Reflectivity and Power Spectral Density of Smoothly Polished Silicon.  LAHSEN ASSOUFID, ALBERT MACRANDEL, SURESH NARAYANAN, RUBEN KHachatRyAN, Argonne, SUNIL SINHA, UCSD — Silicon polished by means of chemical-mechanical-polishing has been studied. A finely crevaced top surface was seen in the AFM data. The power-spectral-density was measured by means of interferometry and by atomic force microscopy, and a roughness value of 0.21 - 0.23 nm rms was found by integration. X-ray reflectivity data for 10 keV x-rays were obtained at the Advanced Photon Source, and a roughness of 0.22 - 0.30 nm was found to be roughly consistent with these data. A surface layer with a slightly higher density than that of crystalline silicon was needed to model the x-ray reflectivety. Crevaces 3.6 nm deep and resulting in land areas having 85% coverage were invoked for the modeling. A total layer thickness of 7.4 nm was invoked for the modeling. That is, the crevaces penetrated roughly half way through the total layer thickness. Due to the overall agreement between the two very different techniques for measuring roughness, namely, PSD and x-ray reflectivity data, we consider these results to accurately quantify roughnesses for a silicon surface that is near the state-of-art for smoothness.

9:36AM A36.00007 Wide-angle incidence x-ray waveguides prepared by micro-/nano-technology using crystal surface diffraction.  SUNG-YU CHEN, National Tsing Hua University, YU-CHI SHEN, MAU-SEN CHIU, CHIA-HUNG CHU, National Tsing Hua University, YURIY P. STETSKO, BO-YUAN SHEW, Nat’l Synchrotron Radiation Research Center, SHIH-LIN CHANG, National Tsing Hua University — Grazing incidence x-ray waveguides have been most studied because of its simple geometry and its applicability for all photon energies. However, wide-angle incidence waveguides are also essential for modern x-ray optics, as far as coupling/guiding x-ray beams into given directions are concerned. To investigate this possibility we have prepared waveguides on silicon wafers by x-ray lithographic technique. The waveguides are 100μm high and 1cm long with different widths and the distance between the adjacent waveguides is 2.5 mm. Both the top and bottom surface of a waveguide are plated with gold. With this type of waveguides we have actually observed the effects of guiding x-rays in both lateral and vertical directions using (113) surface diffraction in Au/Si waveguide systems.

9:48AM A36.00008 Fluctuation electron microscopy studies of complex structured materials.  GONGPU ZHAO, School of Earth and Space Exploration and Department of Chemistry/Biochemistry, Arizona State University, Tempe, AZ, 85287, ANNICK ROUGÉE, Department of Physics, Arizona State University, Tempe, AZ, 85287, PETER BUSECK, School of Earth and Space Exploration and Department of Chemistry/Biochemistry, Arizona State University, Tempe, AZ, 85287, MICHAEL TREACY, Department of Physics, Arizona State University, Tempe, AZ, 85287 — Fluctuation electron microscopy (FEM) is a hybrid imaging-diffraction technique. This technique is particularly sensitive to paracrystalline structures of dimension 0.5-2 nm, which are difficult to detect by either imaging or diffraction techniques alone. It has been successfully deployed to study paracrystalline structures in amorphous silicides, glass, and oxide glasses. This technique has also been used to study metallic glasses and oxide glasses. Until now, FEM has not been used to study disordered geological materials. In this talk we present our FEM studies of shungite, a naturally occurring disordered carbonaceous material, reveal that trace quantities of tightly curved graphene structures such as C60, or fragments of C60, is present in shungite. We also present results from our study of metamict zircon, whose crystal structure is destroyed by self-radiation during naturally occurring α decay events. Work is in progress to study the structural evolution during the metamictization process.

10:00AM A36.00009 Holography with Low Energy Electrons - a New Tool for Structural Biology.  TATIANA LATYCHEVSKAIA, HANS-WERNER FINK, University of Zurich — Holography is widely used for three-dimensional imaging of macroscopic objects using visible light. The same principle can also be applied for imaging of individual molecules like DNA or larger objects, for instance viruses. The holograms are recorded with coherent low energy electrons with wavelength, and thus potential resolution, in the sub-nanometer regime. The experimental setup together with holograms of individual biological molecules and their numerical reconstructions shall be presented. Current experimental and theoretical challenges of holography with low energy electrons will also be addressed. Strong forward scattering of electron waves has been taken into account for the reconstruction process. Since most biological molecules exhibit phase shifting rather than absorbing properties, the retrieval of the phase parallel to the absorbing properties of an object has been realized. On the experimental side, a method towards a significantly improved signal to noise ratio in holograms has been established by acquiring several hundred short pulsed holograms followed by a cross correlation alignment. Finally, the solution to the twin image problem in holography will be presented and reconstructed twin-image free experimental holograms will be shown.

1Supported by the European project SIBMAR.
10:12AM A36.00010 Theory of ultrafast electron diffraction: the role of the pulse properties.1, JOHN SIPE, ANIA MICHALIK, EUGENE SHERMAN, Department of Physics and Institute of Optical Sciences, University of Toronto — We present a general formalism for scattering of electron bunches used in ultrafast electron diffraction (UED) experiments that incorporates characteristic parameters of the incident electron bunch. To perform the scattering calculation, we associate the classical distribution function, which describes the electron bunch just before scattering, with the asymptotic-in Wigner distribution. Using single-scattering and far-field approximations appropriate for typical UED experimental conditions, and considering the effects of the bunch parameters on the scattered signal, we derive two diffraction expressions. We derive a Fraunhofer type expression suitable for scattering from small samples, such as molecules, and a Fresnel type expression appropriate for scattering from large targets such as thin films. In our analysis we also identify the coherence length of an electron bunch. We present sample numerical calculation for scattering by nanosize particles based on our model, and discuss the effects of bunch and scattering target parameters on the diffraction signal.

3We are grateful to the NSERC (Canada) for support.

10:24AM A36.00011 Determination of Adsorbed C_{60} Nanostructures by Low-Energy Electron Diffraction1, M.A. VAN HOVE, G.M. GAVAZA, Z.X. YU, G. XU, S.Y. TONG, City University of Hong Kong, W.W. PAI, C.H. LIN, Center for Condensed Matter Sciences, National Taiwan University — We have recently extended to nanostructures the basic theoretical capabilities of surface structure determination by Low Energy Electron Diffraction (LEED), by adopting a non-periodic cluster approach and substantially accelerating the computation time for complex structures. In this contribution, we describe two further theoretical enhancements and their application to experimental data for buckyballs adsorbed on a Cu(111) surface. One enhancement addresses occasional situations where strong multiple scattering causes poor convergence: this is solved by treating all scattering within subclusters of a few atoms with accurate matrix inversion. Secondly, for the structure determination of complex nanostructures, an efficient search method is essential: for that purpose a modified version of tensor LEED is adapted to nanostructures, called NanoTensorLEED. We exhibit the resulting ability to analyze detailed nanostructures with the case of buckyballs adsorbed on a Cu(111) surface.

1Funded in part by RGC Grant No. CityU1/02C and CityU Grant No. 9610059.

10:36AM A36.00012 RHEED-TRAXS as a tool for in-situ stoichiometry control.1, SANDEEP CHANDRIL, CAMERON KEENAN, THOMAS MYERS, DAVID LEDERMAN, West Virginia University — RHEED-total reflection x-ray spectroscopy (TRAXS) is an in-situ chemical and structural characterization technique which is highly surface sensitive. This consists of a grazing-angle electron beam from which characteristic x-rays from the sample are measured also at grazing angles. We have demonstrated that monolayer sensitivity in Y and Mn films on GaN can be achieved. We have also developed a theoretical model for the angular dependence of the x-ray Kα peaks for the thin films, based on Parratt’s formalism for x-ray reflectivity and the electron trajectory simulation software CASINO, to correct for grazing angle electron beam as a source for x-rays. As the angular dependence is highly dependent upon the film thickness and the smoothness of the film, it can be used to determine the deposition rate of individual elements as well as the interface chemical roughness.

1This work was funded by ONR (Grant N00014-02-1-0974), the AFOSR (MURI grant F49620-03-1-0330), and NSF (CIAM-DMR grant 0502825).

10:48AM A36.00013 First background free measurement of the inelastic tail of the Auger electron spectrum down to 0 eV1, A. H. WEISS, S. MUKHERJEE, M.P. NADESALINGAM, N. G. FAZLEEV, U. Texas at Arlington — Background free measurements of the inelastic tail of the Auger electron energy spectrum were performed by using very low energy positrons to excite Auger transitions in Au and Cu via positron-electron annihilation. The kinetic energy of the incident positrons (1.5eV) was set below the energy threshold required to excite secondary electrons resulting in a Auger spectra that was completely free of collision induced secondary electrons. The measured spectra contain contributions solely from either annihilation induced Auger electrons or annihilation induced Auger electrons that have lost energy on the way out. By using the time of flight technique it was possible to measure the inelastic tail of the Auger electron energy spectrum down to 0 eV.

1Y-1100 Welch Foundation

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Monday, March 10, 2008 8:00AM - 10:48AM —
Session A37 FLAP: Semiconductors I: Growth and Processing Morial Convention Center 229

8:00AM A37.00001 Single phase In_xGa_{1−x}N (0.25 ≤ x ≤ 0.63) alloys synthesized by MOCVD. , BED PANTHA, LI JING, JINGYU LIN, HONGXING JIANG, Kansas State University. KANSAS STATE UNIVERSITY TEAM — In_xGa_{1−x}N alloys have received much attention due to their applications in optoelectronic devices operating in the near infrared region to the near UV region as the band gap of In_xGa_{1−x}N can be continuously tuned from ∼ 0.7 eV (InN) to 3.4 eV (GaN). Recently, it has been suggested that high quality In-rich InGaN alloys offer great potential applications in many important areas as follows: (1) high efficiency multijunction solar cell, (2) high efficiency photoelectrochemical (PEC) cell, and (3) thermoelectric (TE) devices. Our recent experimental results show that In-rich InGaN alloys could be as good as SiGe alloys in terms of figure of merit (ZT) for TE applications. However many experimental techniques have proven that growth of In-rich InGaN alloys is extremely challenging due to the solid phase miscibility gap between InN and GaN. Here we present the growth of single phase InGaN alloys with high In-contents by metal organic chemical vapor deposition on AlN/Al_{2}O_{3} and/or GaN/Al_{2}O_{3} templates. X-ray diffraction was employed to determine indium content. Single peak of wide range theta-2theta scan of (002) plane confirmed that there is no evidence of phase separation. Optical and electrical properties and surface morphology were also studied by photoluminescence, Hall-effect and atomic force microscopy measurements, respectively.

8:12AM A37.00002 High Mobility InN epilayers grown on AlN templates by MOCVD. NEELEM KHAN, ASHOK SEDHAINE, JING LI, JINGYU LIN, HONGXING JIANG, Department of Physics, Kansas State University, Manhattan, KS 66506-2601. — Among III-nitrides, InN has the smallest electron effective mass, the largest mobility and smallest direct band gap. These distinguished properties make InN an interesting material for applications in high speed electronic devices and full color displays. However, obtaining InN and In-rich InGaN epilayers with controllable conductivity is still a challenging task. We report here on the growth and transport property studies of InN epilayers on AlN templates, as compared to GaN templates. Significant improvements in the electrical and optical properties of InN epilayers were observed on AlN templates. A Hall mobility of 1390 cm^2/Vs with a carrier concentration of 1x10^{19}cm^{-3} at room temperature was observed, which is highest value reported for MOCVD grown InN epilayers. The photoluminescence emission spectra revealed band to band emission peak at ∼0.75 eV. The effects of post growth annealing on transport, structural and optical properties of undoped and Mg-doped InN epilayers will also be presented.
Si nanomembranes with mixed crystal orientations

SHELLEY SCOTT, DEBORAH COTTRELL, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin-Madison — Higher-carrier-mobility CMOS devices enhance processor speed. The large mobilities that have a form of the lognormal type. The resulting expression is used to discuss the grain size distribution of solid phase crystallized Si-films.

time development of grain size distribution in random nucleation and growth processes. The solution of this equation provides an analytical derivation of size distributions that has a form of the lognormal type. The logarithmic-normal (lognormal) distribution is one of the most frequently observed distributions in nature and describes a large number of physical, biological, and technological processes. The lognormal distribution is often used in modeling phenomena where the logarithm of the variable follows a normal distribution.

BERGMANN, Robert Bosch GmbH, Automotive Electronics, Quality Management Suppliers, Physical Analysis, P.O.Box 1342, 72703 Reutlingen, Germany — The need to develop reliable and cost-effective alternatives to solid-state devices is rapidly growing. Solar light is among the most important and promising, therefore new materials are searched for to effectively overlap and harvest the solar spectrum. Here we describe the preparation of titanium oxide nano-clusters utilizing amorphous solid water (ASW) as a reactive buffer layer to assist the growth of titanium oxide clusters. These clusters were grown in-vacuum on top of ASW layers at 120K. Upon evaporation of the water layer, seed Ti(OH)$_n$ clusters polymerize via a solid-state "Sol-Gel-like" mechanism. Self-termination process, dictated by the evaporated water vapor, results in hemispherical clusters 5-7 nm in diameter. The clusters were analyzed by XPS at 300K. The clusters grown this way were studied by employing 4K photoluminescence spectroscopy, revealing a typical diode-like I-V profile. An apparent band gap of 2.3-2.5 eV was obtained, significantly narrower than the bulk value of TiO$_2$ crystal (3.2 eV). Thermal stability of these defect rich clusters need to be studied, since this may prove important for photocatalysis and photovoltaic applications.

8:24AM A37.00003 Growth of the BN – nanostructured materials using borazine decomposition by Laser Chemical Vapor Synthesis, ARTURO HIDALGO, VLADIMIR MAKAROV, DACHUN HUANG, GERARDO MORELL, BRAD WEINER — We describe BN nanostructured materials growth by Laser Chemical Vapor Synthesis (LCVS) using the precursor borazine B$_3$N$_6$H$_6$. As a result due to laser induced creation of the active chemical intermediates in the bulk volume, and further development of the "dark" chain processes in the borazine vapor with formation of the BN nano-tubes and hydrogen gas. The phenomenological model qualitatively describing the observed phenomenon was developed and applied to explanation of the studied effects. The variation of radiation density (J/cm$^2$) for both harmonics and pressure is used for optimized the amount obtained.

8:36AM A37.00004 Anomalous Coherent Bragg Rod Analysis Studies of GaAs/InGaAs. DIVINE KUMAH, NAJI HUSSENI, CODRIN CIONCA, ALEX RIPOSAN, Applied Physics Dept. University of Michigan, JOANNA MIRECKI MILLUNICH, Department of Materials Science and Engineering, University of Michigan, PHIL WILLMOTT, ROY CLARKE, Swiss Light Source, YIZHAK YACOBY, Racah Institute of Physics, Hebrew University — A considerable amount of work has been carried out recently in correlating growth conditions with electronically observed properties of Group III-V systems using a variety of characterization techniques. Ambiguity in interpretation of most characterization techniques arises due to difficulties in separating roughness effects from segregation and inter-diffusion of atomic species. We apply x-ray resonant techniques to the Coherent Bragg Rod Analysis (COBRA) phase retrieval procedure to produce high resolution electron density maps from bragg rod scans to determine with a high degree of accuracy, the relative concentrations of In and Ga in a system comprising of 1ML of GaAs on InGaAs.

8:48AM A37.00005 Growth and Characterization of Non-Polar, A-Plane ZnO Thin Films, PRIYA V. CHINTA, O. LOZANO, P. WADEKAR, L.H. CHU, Q.Y. CHEN*, W.K. CHU, Texas Center for Superconductivity and Dept. of Physics, University of Houston, TX, H.W. SEO, Department of Physics, University of Arkansas, AR, L.W. TU, N.J. HO, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, NSYSU, Taiwan. — The growth and characterizations of non-polar a-axis-oriented epitaxial films of ZnO deposited by magnetron sputtering were investigated in comparison with the polar c-axis-oriented counterparts. The single-phase a-axis-oriented films were obtained at 700-degree C substrate temperature, whereas both a- and c-axis orientations were observed when deposited at lower temperatures ranging from 400 degree C to 600 degree C. The structural, morphological and temperature effects on photoluminescence behaviors have been studied. X-ray rocking curves show that the FWHM of (11-20) peak increases with temperature up to 600 degree C but start to decreases beyond 700C. Atomic force microscopy reveals significant changes in surface morphology as the growth temperature varies. Optical properties of the differently oriented films will be presented. PL emission in UV range was observed for the a-plane ZnO films which has been attributed to neutral donor bound exciton. The effect of Al-doping will also be discussed. *Also with NSYSU.

9:00AM A37.00006 Pinpoint Growth Mechanism Of ZnO Nanoparticles, DA-JUN SHU, XIANG XIONG, MU WANG, National Laboratory of Solid State Microstructures and Department of PhysicsUniversity, Nanjing University, Nanjing 210093, China, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES AND DEPARTMENT OF PHYSICSUNIVERSITY COLLABORATION — We investigate the growth mechanism of ZnO nanoparticles synthesized by thermal evaporation method. Temperature is tuned to control the growth driving force while other conditions are fixed. Classical nucleation theory and growth dynamics are used to analyze the competition between growth in lateral and vertical directions. Interfacial diffusion properties, step edge diffusion barrier and several other factors affecting the growth of nanostructures are taken into account. Based on these considerations we have established a model which suggests a quantitative relation between temperature and the size of nanoparticles. Programmed cooling processes are introduced into the thermal evaporation to verify the theoretical expectations. It is also demonstrated that a morphology-controllable hierarchical prisms, which is expected from our theoretical model, can be easily achieved by tuning the temperature. The authors acknowledge the financial support from the Ministry of Science and Technology of China (Grants No.2004CB119005 and No.2006CB801004).

9:12AM A37.00007 Titanium oxide nano-clusters prepared via amorphous solid water: Improved overlap with solar spectrum, MICHA ASCHSER, The Hebrew University of Jerusalem — The need to develop reliable and cost-effective alternative energy sources is rapidly growing. Solar light is among the most important and promising, therefore new materials are searched for to effectively overlap and harvest the solar spectrum. Here we describe the preparation of titanium oxide nano-clusters utilizing amorphous solid water (ASW) as a reactive buffer layer to assist the growth of titanium oxide clusters. These clusters were grown in-vacuum on top of ASW layers at 120K. Upon evaporation of the water layer, seed Ti(OH)$_n$ clusters polymerize via a solid-state "Sol-Gel-like" mechanism. Self-termination process, dictated by the evaporated water vapor, results in hemispherical clusters 5-7 nm in diameter. The clusters were analyzed by XPS at 300K. The clusters grown this way were studied by employing 4K scanning tunneling spectroscopy, revealing a typical diode-like I-V profile. An apparent band gap of 2.3-2.5 eV was obtained, significantly narrower than the bulk value of TiO$_2$ crystal (3.2 eV). Thermal stability of these defect rich clusters need to be studied, since this may prove important for photocatalysis and photovoltaic applications.

9:24AM A37.00008 On the logarithmic-normal distribution in nucleation and growth processes, ANDREAS BILL, ANTHONY TERAN, California State University Long Beach, Dept. of Physics & Astronomy, Long Beach, CA 90840-3901, RALF B. BERGMANN, Robert Bosch GmbH, Automotive Electronics, Quality Management Suppliers, Physical Analysis, P.O.Box 1342, 72703 Reutlingen, Germany — The logarithmic-normal (lognormal) distribution is one of the most frequently observed distributions in nature and describes a large number of physical, biological and even societal phenomena. However, a deviation of this distribution from first principles is lacking. We propose a differential equation governing the time development of the size distribution in random nucleation and growth processes. The solution of this equation provides an analytical derivation of size distributions that has a form of the lognormal type. The resulting expression is used to discuss the grain size distribution of solid phase crystallized Si-films.

9:36AM A37.00009 Si nanomembranes with mixed crystal orientations, SHELLEY SCOTT, DEBORAH COTTRELL, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin-Madison — Higher-carrier-mobility CMOS devices enhance processor speed. Carrier mobility can be optimized by fabricating mixed regions of Si(110) (high hole mobility) and Si(001) (high electron mobility) on a single substrate, so-called hybrid-orientation technology (HOT). We fabricate a mixed-crystal-orientation material using Si nanomembrane (SiNM) transfer and overgrowth. The top Si layer of SOI(110) is patterned with an array of holes and removed from its handle substrate, creating a Si(110)NM, which is then bonded to Si(001). We deposit Si over the structure with CVD, which is much faster on Si(001) than on Si(110), allowing planarization of the surface (i.e., hole filling), to produce a flat mesh of Si(001) and Si(110) regions. We characterize the mesh with XRD, SEM, and AFM. We can fabricate HOT membranes for transfer to various (including flexible) substrates, and can incorporate strain to tune mobilities. With strained Si(110)NMs, we expect a hole mobility enhancement of ~70% over Si(001) while maintaining the high electron mobility of Si(001), thereby dramatically reducing the mobility imbalance between n- and p-type devices. Supported by DOE and NZFRST.
9:48AM A37.00010 Strain Relaxation in Elastically Strain-Sharing Silicon (110) Nanomembranes1, DEBORAH COTTRILL, SHELLEY SCOTT, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin-Madison. — TEAM — Tensely strained Si(110) has potential for advanced CMOS and p-MOS devices because, depending on strain and current direction, hole mobility can be increased to 150% of that of unstrained Si(110) and an electron mobility nearly equal. Previous efforts to strain Si(110) tensely have relied on the formation of partial dislocations for strain relaxation, resulting in large asymmetric components of the in-plane strain and high threading dislocation densities, which alter device performance. We use thin multi-layer heterostructures of Si/SiGe/Si(110) grown with MBE on Si(110)-on-insulator that elastically strain share when released from the handling substrate. Besides their very high flexibility, these nanomembranes (NMs) are virtually dislocation free and exhibit a lower degree of asymmetric in-plane strain relaxation than achieved with threading dislocation relaxation; the NMs rely on elastic strain transfer rather than partial dislocation propagation. We use AFM, XRD, and Raman to characterize growth, strain transfer, and strain anisotropy.

1Supported by AFOSR DOE, NDSEG Fellowship (DMC), and NZFRST Fellowship (SAS).

10:00AM A37.00011 A Novel Route for the Synthesis of Graphene by Microwave Plasma Enhanced Chemical Vapor Deposition, ALEXANDER MALESEVIC, MANISH PAL CHOWDHURY, LIANG ZHANG, ANNIK VAN-HULSEL, CHRIS VAN HAESENDONCK — A novel route for the synthesis of graphene by means of microwave plasma enhanced chemical vapor deposition is presented. This technique outclasses its competitors in many ways since it is less elaborate and better reproducible than micromechanical cleavage of graphite and less expensive than thermal decomposition of silicon carbide wafers. Methane diluted with hydrogen is decomposed in a high power microwave plasma and the resulting carbon radicals recombine on the surface of any substrate that withstands temperatures up to 700 °C. A broad range of substrates were successfully tested including silicon, quartz, stainless steel and many metals. The resulting carbon nanostructures are freestanding graphene flakes, only four to six atomic layers thick but up to several micrometers wide and high. The flakes are perpendicular aligned to the substrate surface. Thorough qualitative analysis lead to the conclusion that the flakes are highly crystalline sp2 carbon nanostructures with few defects or impurities. A possible growth scheme is proposed and field emission measurements of as grown flakes reveal a low turn on voltage of only 3V/µm which is a promising value for possible future applications.

10:12AM A37.00012 Structure of Iron Silicon Germanide and Osmium Silicide Epitaxial Films Measured by X-Ray Absorption Spectroscopy1, NADER ELMARHOUMI, R. COTTIER, F. AMIR, Univ. of North Texas, G. MERCCHAN, A. ROY, CAMD/LSU, H. GEISLER, C. A. VENTRICE JR., T. D. GOLDING, Texas State Univ. — Some of the iron- and osmium-based metal silicide and germinide phases have been proposed to be direct band gap semiconductors. We have used synchrotron-based x-ray absorption spectroscopy to study the structure of iron silicon germanide and osmium silicon silicide films grown by molecular beam epitaxy. Osmium silicide films which are primarily in the Os5Si3 phase and a series of Fe(Si1−xGex)2 films with a nominal Ge concentration of up to x = 0.04 have been grown. X-ray absorption near edge structure (XANES) measurements on both the iron silicon germinide and osmium silicide films have been performed. An absorption edge shift of 0.9 eV is observed for the osmium silicide films; however, no shift was observed for the iron silicon germinide films. Extended x-ray absorption fine structure (EXAFS) measurements have also been performed on the iron silicon germinide films. The nearest neighbor coordination corresponding to the β-FeSi phase of iron silicide provides the best fit with the EXAFS data.

1This work was supported in part by ONR.

10:24AM A37.00013 Studies of the Ge(100) Surface Using a Low Energy Positron Beam: The Effects of Surface Reconstructions on Positron Trapping and Annihilation Characteristics, N. G. FAZLEEAA, A. H. WEISS, Department of Physics, University of Texas at Arlington — Positron annihilation induced Auger electron spectroscopy (PAES) has been applied to study the Ge(100) surface. The PAES spectrum from the Ge(100) surface displays several strong Auger peaks corresponding to M4.5N1N2,3, M2.3M4.5M4.5, M2.3M4.5V, and M1M4.5M4.5 Auger transitions. The integrated peak intensities of Auger transitions are used to obtain experimental annihilation probabilities for the Ge 3d and 3p core level electrons. The experimental results are analyzed by performing calculations of positron surface states and annihilation characteristics of surface trapped positrons with relevant Ge core-level electrons for the reconstructed Ge(100)-p(2x1), Ge(100)-p(2x2), and Ge(100)-c(4x2) surfaces. The PAES spectrum from the Ge(100) surface displays several strong Auger peaks corresponding to M4.5N1N2,3, M2.3M4.5M4.5, M2.3M4.5V, and M1M4.5M4.5 Auger transitions. The integrated peak intensities of Auger transitions are used to obtain experimental annihilation probabilities for the Ge 3d and 3p core level electrons. The experimental results are analyzed by performing calculations of positron surface states and annihilation characteristics of surface trapped positrons with relevant Ge core-level electrons for the reconstructed Ge(100)-p(2x1), Ge(100)-p(2x2), and Ge(100)-c(4x2) surfaces. Estimates of positron binding energy, work function, and annihilation characteristics reveal their sensitivity to surface reconstruction of the topmost layers of clean Ge(100). These results are compared to the ones obtained for the reconstructed Si(100)-(2x1) and Si(100)-(2x2) surfaces. A comparison with PAES data reveals an agreement with theoretical core annihilation probabilities for the Auger transitions considered.

10:36AM A37.00014 X-ray Photoelectron Spectroscopic Investigation of Oxidation of Hafnium1, JOHN HICKMAN, STEVEN MCDONOUGH, R.L. MILLER, M.A. SEABOLT, G.A. NIXON, A.R. CHOURASIA, Department of Physics, Texas A&M University-Commerce — X-ray photoelectron spectroscopy has been employed to investigate the oxidation of hafnium. Thin films (20 Å) of elemental hafnium were deposited on silicon substrates using e-beam technique. Two types of samples were investigated. In one type, the substrate was annealed at the desired temperature after the deposition. In the other type, the substrate was kept at the desired temperature during the deposition. The substrate temperatures were kept at 100, 200, 300, 400, 500, and 600 °C. Hafnium is observed to get deposited mostly as hafnium dioxide with some suboxide. The amount of the suboxide is found to vary with the processing conditions. The concentration of the dioxide and the suboxide were determined by curve fitting the spectra. The fitting was performed using the parameters determined from fitting pure elemental hafnium spectrum and pure hafnium dioxide spectrum.

1Supported by Research Corporation and Organized Research, TAMU-Commerce.

Monday, March 10, 2008 8:00AM - 10:24AM — Session A38 DBP DMP: Focus Session: Biocompatibility Morial Convention Center 230
8:00AM A38.00001 The quantification of biocompatibility: toward a new definition, BUDDY RATNER, University of Washington — Implantable medical devices, and the biomaterials that comprise them, form a $100B business worldwide. Medical devices save lives and/or improve the quality of life for millions. Tissue engineering also makes extensive use of biomaterials—biomaterials are an enabling technology for tissue engineering. A central word to understanding the effectiveness of such materials and devices is biocompatibility. The word “biocompatible” is widely used in reference to biomaterials and medical devices and most everyone has some value understanding of its meaning. Many formal definitions have been proposed for this word, but it is still largely used in an imprecise manner. Four descriptions or definitions of biocompatibility will be reviewed: a widely adopted definition from a consensus conference, a surgeon’s perspective on this word, the regulatory agency view, and the factors that clearly influence biocompatibility. In this talk, the classical definition of biocompatibility will be contrasted to a newer definition embracing molecular concepts and the understanding of normal wound healing. The biological data on the in vivo healing responses of mammals to implants will be described. A strategy to improve the healing of biomaterials will be presented. It is based upon surface molecular engineering. First, non-specific protein adsorption must be inhibited. Strategies to achieve this design parameter will be presented. Then methods to deliver the specific protein signals will be addressed. Matricellular proteins such as osteopontin, thrombospondin 2 and SPARC will be introduced with an emphasis on exploiting the special reactivity of such proteins. A discussion of the influence of surface textures and porosities will also be presented. Finally a new scheme based upon macrophage phenotypic pathways will be proposed that may allow a quantitative measure of extent of biocompatibility.

1Support was received from the UWEB NSF Engineering Research Center

8:36AM A38.00002 Biocompatibility of implantable biomedical devices, SUPING LU, Medtronic Inc — Biomedical devices have been broadly used to treat human disease, especially chronic diseases where pharmaceuticals are less effective. Heart valve and artificial joint are examples. Biomedical devices perform by delivering therapies such as electric stimulations, mechanical supports and biological actions. While the uses of biomedical devices are highly successful they can trigger adverse biological reactions as well. The property that medical devices perform with intended functions but not causing unacceptable adverse effects was called biocompatibility in the early time. As our understanding of biomaterial-biological interactions getting broader, biocompatibility has more meanings. In this talk, I will present some adverse biological reactions observed with implantable biomedical devices. Among them are surface fouling of implantable sensors, calcification with vascular devices, restenosis with stents, foreign particle migration and mechanical fractures of devices due to inflammation reactions. While these effects are repeatable, there are very few quantitative data and theories to define them. The purpose of this presentation is to introduce this biocompatibility concept to biophysicists to stimulate research interests at different angles. An open question is how to quantitatively understand the biocompatibility that, like many other biological processes, has not been quantified experimentally.

9:12AM A38.00003 A Gaussian theory of the response of heart frequency to ventilator, YAN LU, MICHAEL DEEM, Rice University, ANTON BURYKIN, TIMOTHY BUCHMAN, Washington University School of Medicine, RICE UNIVERSITY TEAM, WASHINGTON UNIVERSITY SCHOOL OF MEDICINE TEAM — Extensive studies suggest that there exists a coupling between the human heart and respiration. We studied changes in cardio-respiratory synchrony and dynamics of cardiovascular system during transition from mechanical ventilation to spontaneous respiration in critically ill patients. This observational study exploits a standard clinical practice—the spontaneous breathing trial (SBT). The SBT consists of a period of mechanical ventilation, followed by a period of spontaneous breathing, followed by resumption of mechanical ventilation. We collected continuous respiratory, cardiac (EKG), and blood pressure signals of mechanically ventilated patients before, during and after SBT. The data were analyzed by means of spectral analysis, phase dynamics, and entropy measures. Mechanical ventilation appears to affect not only the lungs but also the cardiac and vascular systems. Spontaneous cardiovascular rhythms are entrained by the mechanical ventilator and are drawn into synchrony. Sudden interruption of mechanical ventilation causes gross desynchronization, which is restored by reinitiation of mechanical ventilation. The data suggest (1) therapies intended to support one organ system may propagate unanticipated effects to other organ systems and (2) sustained therapies may adversely affect recovery of normal organ system interactions.

9:24AM A38.00004 Synchronization of Cardio-Respiratory Dynamics in Critically Ill Patients, ANTON BURYKIN, TIMOTHY BUCHMAN, Washington University in St. Louis — We studied changes in cardio-respiratory synchrony and dynamics of cardiovascular system during transition from mechanical ventilation to spontaneous respiration in critically ill patients. This observational study exploits a standard clinical practice—the spontaneous breathing trial (SBT). The SBT consists of a period of mechanical ventilation, followed by a period of spontaneous breathing, followed by resumption of mechanical ventilation. We collected continuous respiratory, cardiac (EKG), and blood pressure signals of mechanically ventilated patients before, during and after SBT. The data were analyzed by means of spectral analysis, phase dynamics, and entropy measures. Mechanical ventilation appears to affect not only the lungs but also the cardiac and vascular systems. Spontaneous cardiovascular rhythms are entrained by the mechanical ventilator and are drawn into synchrony. Sudden interruption of mechanical ventilation causes gross desynchronization, which is restored by reinitiation of mechanical ventilation. The data suggest (1) therapies intended to support one organ system may propagate unanticipated effects to other organ systems and (2) sustained therapies may adversely affect recovery of normal organ system interactions.

9:36AM A38.00005 Crystal Structure Properties of Human Teeth as a Function of Age, TH. LEVENTOURI, A. KYRIACOU, R. VENTURELLI, A. ANTONAKOS, E. LIAROKAPIS, V. PERDIKATSIS, Florida Atlantic University — We report on crystal structure studies of human teeth as a function of age in the range of 5-87 years. The crystallinity of the hydroxyapatite, which is the main dental mineral phase in teeth, decreases with age in a systematic way starting at ~40 years old teeth. The average crystallite size decreases from ~40 nm to ~12 nm in the age range 30 to 60 years old and then it remains practically constant. The a-lattice constant decreases in a similar systematic way and it is associated with the carbonate content of the tooth. Development of the secondary phases with the tooth-age questions the crystallographic structure of the dental apatite. FTIR spectroscopy reveals both types of carbonate substitution, but B-type substitution is greater by a factor of 4 than the A-type. An increase of the carbonate content with the tooth age is also deduced from the ratio of the V2 CO3 to the V1 PO4 IR modes from 17 to 70 years of age. TGA measurements confirm the results of both experimental methods.

1Support from the Cancer Institute at the FAU Research Park is acknowledged.

9:48AM A38.00006 Procedure to Measure Effect of Excess Body Mass on Musculoskeletal: II. Implementation, SAAMI J. SHAIBANI, Independent Modeling, Algorithms & Analytical Studies (IMAAS) — There are a number of ways in which the musculoskeletal system can be affected by excess body mass. One representative quantity for these is the torque exerted on the spinal column about a horizontal lateral axis; hence, its use as an illustrative mechanical indicator in the research reported here. Values of the torque are determined for all subjects in an exceptionally broad adult population that was developed during a companion study. Increases in body mass index caused nearly uniform increases in torque for all height percentiles in both sexes. Overweight individuals had torques that were 35 and 30 percent greater (females and males, respectively) than those for healthy individuals of the same height. Corresponding increases for obese individuals occurred at the much higher levels of 75 and 66 percent. Any resulting musculoskeletal damage from this is in addition to other problems arising from obesity, such as heart disease, diabetes, and high blood pressure. However, whereas the latter can be treated or managed with medication, some facets of the former might be irreversible and/or irremediable.
10:00AM A38.00007 Extremely high paw accelerations during paw shake in the cat: A mechanism revealed by computer simulations. ALEXANDER KLISHKO, Georgia Tech USA; Inst of Math Problems of Biol Puschino Russia. DAVID COFER, DONALD EDWARDS, Georgia State University; BORIS PRILUTSKY, Georgia Tech, GEORGIA TECH TEAM, GEORGIA STATE UNIVERSITY COLLABORATION — Paw shake response is a reflex aimed at removing an offending stimulus from the paw by imparting to it high periodic accelerations (≥10 g). These values seem too high to be produced by distal muscles exclusively. According to Prilutsky et al. (2005), resultant hip moments during paw shake are much greater than distal joint moments, whereas distal joint velocities and accelerations exceed those of the proximal joints. The goal of this study was to examine how proximal hip muscles could contribute to high paw accelerations. Using software AnimatLab, we developed a 2D model of the cat hindlimb consisting of 5 rigid segments with 4 hinge joints and 11 muscles spanning all joints. The muscles were assumed passive except for those crossing the hip. When in simulations the hip muscles were reciprocally activated to periodically flex and extend the hip joint with a typical paw shake frequency of 10 Hz, the hindlimb segments demonstrated motion resembling experimental observations: linear and angular velocities and accelerations of the distal segments exceeded several fold the values of the proximal segments. Simulated paw shake revealed features of a whip-like motion.

Monday, March 10, 2008 8:00AM - 11:00AM — Session A39 GSNP: Focus Session: Elasticity and Geometry of Thin Objects Morial Convention Center 231

8:00AM A39.00001 Delamination of thin elastic sheets from soft, sticky substrates. DOMINIC VELLA, LPS ENS, PEDRO REIS, Department of Mathematics, MIT; DENIS BARTOLO, JOSE BICO, PMMH, ESPCI; ALEXZK BOUDAOU, LPS ENS, BENOIT ROMAN, PMMH, ESPCI — We study the compression of a soft elastic substrate with a thin sheet adhered to its surface. In this situation, it is energetically expensive for the thin sheet to alter its length. Instead, it accommodates its excess length by delamination from the substrate, allowing it to bend out of the plane. Rather than forming a single ‘blister’, however, we observe the formation of several blisters with a characteristic size. Here, we investigate the dependence of this characteristic blister size on the material properties of the system using a combination of experimental and theoretical analyses.

8:12AM A39.00002 The frustrating tearing of adhesive tape. BENOIT ROMAN, PMMH UMR7636 CNRS/ESPCI; Paris6, Paris 7, EUGENIO HAMM, Departamento de Fisica, Universidad de Santiago de Chile. PEDRO M. REIS, Department of Mathematics, M.I.T.; M. LEBLANC, University of Chicago, ENRIQUE CERDA, Departamento de Fisica, Universidad de Santiago de Chile — When trying to remove an adhesive tape, one often only manages to peel off a useless pointy strip: the fracture tips on both sides of the pulled strip seem to attract each other, and merge in a finite distance. Why don’t they repel each other and lead to a continually increasing width of the strip, as one would like to? We will present an experimental and theoretical study of this pinch-off phenomenon in the rupture of peeled adhesive sheets. The cut shapes are very reproducible, and we will show that the geometry of the peeling field, where elastic energy is concentrated, plays a major role here.

8:24AM A39.00003 Instability of an elastic knot under twist. BASILE AUDOLY, CNRS / University Paris 6, NICOLAS CLAUVELIN, Universite Paris 6, SEBASTIEN NEUKIRCH, CNRS / University Paris 6, INSTITUT DE MECANIQUE D’ALEMBERT TEAM — In a recent paper, we derived a solution to the Kirchhoff equations representing a knotted elastic rod held by a tensile force applied at its ends. This problem has been formulated as the minimization of a curvature energy in the presence of a topological constraint. We extend this analysis to the case of a knot subjected to both a tensile force and a twisting moment. We unveil a striking instability that can be easily reproduced with a piece of computer cord: a simple knot, initially comprising a loop merging with a localized brad, can be unfolded under applied twist into a symmetric shape resembling the figure of eight. Doing so, it becomes much easier to untie.

8:36AM A39.00004 On the statistical physics of folding and crumpling. AREZK BOUDAOU, LPS CNRS/Ecole Normale Superieure — Unfolding a ball of crumpled paper reveals numerous ridges with a wide distribution of sizes. How can we describe the statistics of sizes and energies? Can we understand this system using the tools of statistical physics? During my talk, I will review the various experimental and theoretical approaches that we used to tackle these questions, which are typical of glasses and granular media.

9:12AM A39.00005 The Shape of the Optimal Javelin. YOSSI FARJOUN, MIT, JOHN NEU, UC Berkeley — To find the shape of a javelin whose vibrations dampen the fastest, we seek to maximize the eigenvalue of the first eigen-mode of a vibrating rod. The problem is related to (and is inspired by) the classical problems of finding the tallest and strongest columns solved by J. B. Keller [1], and J. B. Keller and F. I. Norisron [2]. A 4th order ODE for the maximizing eigen-mode is readily solved, however it is ill-conditioned at the boundaries, and standard numerical methods fails. Using a similarity solution, we “peel away” the singularity, and solve the remaining part “backwards”. The resulting shape has a frequency of vibration 5 times larger than that of the uniform-diameter rod. The method of solution is applicable to other similar problems. For example, we confirm the shape of the tallest column with it. [1] The Strongest Column / J. B. Keller ; Arch. Rat. Mech. Anal. 1960 (5), pp. 275–285

9:24AM A39.00006 Impacts on thin elastic sheets. ROMAIN VERMOREL, NICOLAS VANDENBERGHE, EMMANUEL VILLERMUAY, IRPHE - Aix Marseille Université, FRAGMENTATION AND MIXING TEAM TEAM — The radial cracks developing from the impact point of a projectile on a windscreen are of common experience. We investigate the origin of this phenomenon using thin elastic sheets as an experimental model. A projectile launched at controlled speed impacts a free membrane at rest. A tensile front set off from the point of impact and propagates radially at the speed of sound. Flexural waves can propagate in the extended area. Specifically, the interaction between the rigid body and the elastic sheet gives birth to a conical flexural wave whose base expands radially at a well defined velocity. During the propagation of both the tensile and flexural fronts, the radial tensile stress field results in a compressive stress in the azimuthal direction, which triggers a buckling instability. That instability is responsible for the formation of radial folds, with a well defined azimuthal wave number. Based on detailed experimental observations and measurements, we propose a model to understand the wave motion and stress field consequent to the impact; in addition, we provide a prediction for the number of folds selected during the buckling instability as a function of the relevant parameters, including impact velocity.
We acknowledge financial support from NSF-DMR 0606216 and NSF-CBET 0609107

1 SCAT project and the ALFA Programme of EuropeAid.
2 Universidad de Santiago de Chile

9:36AM A39.00007 Spiraling Cracks in Thin Sheets¹, VICTOR ROMERO², BENOIT ROMAN, PMMH CNRS, ENRIQUE CERDA, Universidad de Santiago de Chile — A wide kind of everyday-life industrial products come in a thin package that needs to be torn open by the user, and the opening is not always easy. We built a simple setup to study crack propagation in thin sheets coupled with large out-of-plane displacement: A cylindrical tool is inserted in a straight incision in a thin sheet, and is pushed against the sheet perpendicularly to that incision, eventually propagating a crack. When the blunt tool is continually pushed against the lip, we found that the crack follows a very robust spiraling path. Experiments may be interpreted in terms of “Spira Mirabilis” (logarithmic spiral). Starting with crack theory argument, we will show that the early behavior of the cut path follows a portion of a logarithmic spiral, and that the path tends to another spiral with a different pitch as the crack adds more turns. Our crack experiment illustrates the fact that thin sheets mechanics is deeply connected to geometry, and finally spirals characteristics allow us to measure material crack properties of the thin layer used.

¹SCAT project and the ALFA Programme of EuropeAid.
²Universidad de Santiago de Chile

9:48AM A39.00008 Interaction Between Two Localized Wrinkle Patterns, JIANGSHUI HUANG, WIM H. DE JEU, NARAYANAN MENON, THOMAS P. RUSSELL, Department of Physics, Polymer Science and Engineering, University of Massachusetts Amherst — A drop of water placed on the surface of a freely floating ultrathin polymer film produces a radial wrinkling pattern due to the capillary force it exerts on the film. We have previously characterized the number N and length L of the wrinkles. We now study the interaction between two such localized wrinkling patterns each induced by one drop of water. The patterns distort, and radial symmetry about each drop is lost, with the wrinkles extending further along the line between the drops. When the drops are brought closer, a single long wrinkle forms along this axis. We use the distance at which this connecting wrinkle appears to quantify the range of the interaction between the wrinkles. We will present data for this interaction length as a function of other length scales in the experiment. 1. Full reference here. Science 317, 650(2007)

10:00AM A39.00009 Pattern transformation triggered by deformation,¹ TOM MULLIN, University of Manchester — Periodic elastomeric cellular solids are subjected to uniaxial compression and novel transformations of the patterned structures are found upon reaching a critical value of applied load. The results of a numerical investigation reveal that the pattern switch is triggered by a reversible elastic instability. Excellent quantitative agreement between numerical and experimental results is found and the transformations are found to be remarkably uniform across the samples. Moreover the phenomenon is found to be robust for a range of soft solids including rubber and jelly. *Joint work with M.C. Boyce, K. Bertoldi and S. Deschanel, MIT.

¹EPSRC

10:12AM A39.00010 Granular Silo collapse: an experimental study,¹ ERIC CLEMENT, ESPCI-Universite Paris 6, GUSTAVO GUTIERRIEZ, Departamento de Fisica, Universidad Simon Bolivar, Caracas, Venezuela, PHILIPPE BOLTENHAGEN, boltenhagen@pmmh.espci.fr, JOSE LANUZA, ESPCI-Universite Paris 6 — We present an experimental work that develop some basic insight into the pre-buckling behavior and the buckling transition toward plastic collapse of a granular silo. We study different patterns of deformation generated on thin paper cylindrical shells during granular discharge. We study the collapse threshold for different bed height, flow rates and grain sizes. We compare the patterns that appear during the discharge of spherical beads, with those obtained in the axially compressed cylindrical shells. When the height of the granular column is close to the collapse threshold, we describe a ladder like pattern that rises around the cylinder surface in a spiral path of diamond shaped localizations, and develops into a plastic collapsing fold that grows around the collapsing silo.

¹Progran PCP-France-Venezuela

10:24AM A39.00011 Sudden ridge collapse in the stress relaxation of thin crumpled polymer films, INGO DIERKING, PAUL ARCHER, University of Manchester — Uniform compression of thin crumpled sheets subjected to a constant weight has been shown to exhibit a remarkably wide range of scaling behaviour, covering up to five orders of magnitude [1], i.e. time scales from seconds to weeks. We demonstrate that this scaling behaviour is not smooth, but rather interrupted by sudden changes in height of the uniformly compressed crumple, which we attribute to sudden ridge collapses. The height of the discontinuous jumps due to sudden ridge collapse during the compression process increases with increasing thickness of the polymer film. This is attributed to the fact that thick films exhibit a smaller defect density, but increased defect length. Interestingly, when plotting the time laps between successive ridge collapses as a function of time, the data collapses to a single line for all film thicknesses, with a slope of $d\Delta t/dt=1$ over a scaling regime of four orders of magnitude. Possible explanations will be discussed. [1] K. Matan, R.B. Williams, T.A. Witten, S.R. Nagel, Phys. Rev. Lett., 88, (2002), 076101.

10:36AM A39.00012 Geometry, mechanics and statistical physics in crumpled structures, LAURENT BOUE, AREZKI BOUDAOU, MOKHTAR ADDA-BEDIA, STÉPHANIE DEBOEUF, EYTAN KATZAV, Laboratoire de Physique Statistique, ENS Paris — There’s been a recent surge of interest in the study of low-dimensional packed elastic manifolds. In fact, the simple act of crumpling a piece of paper does require the simultaneous interaction of many fascinating mechanisms. These include energy condensation from large length scales to small singular topological self-avoidance and complex phase space landscapes reminiscent of frustration in the context of glassy systems. We will present a numerical experiment modeling the folding of an elastic rod (1D) restricted to a shrinking 2D space. The confinement is obtained by preparing an initially disordered elastic line embedded in a quadratic potential. Varying the strength of this confining potential shows that many metastable states can be observed. We are reaching a critical value of applied load. The results of a numerical investigation reveal that the pattern switch is triggered by a reversible elastic instability. Excellent quantitative agreement between numerical and experimental results is found and the transformations are found to be remarkably uniform across the samples. Moreover the phenomenon is found to be robust for a range of soft solids including rubber and jelly. *Joint work with M.C. Boyce, K. Bertoldi and S. Deschanel, MIT.

10:48AM A39.00013 Inside a Ball of Crumpled Aluminum Foil,¹ ANNE DOMINIQUE CAMBOU, NARAYANAN MENON, UMass Amherst — We have studied the three-dimensional geometry of a crumpled sheet via x-ray CT scans. We crumple circular sheets of aluminum with thicknesses of 30-50µm and diameter 100000µm into spherical balls of diameter 15000-20000µm. We then perform CT scans with a resolution of 6µm³/voxel. This allows us to fully resolve the conformation of the sheet. We use the reconstructed CT images to determine the mass distribution inside the crumpled ball. We also report on a box-counting analysis to assess the fractal nature of the mass distribution.

¹We acknowledge financial support from NSF-DMR 0606216 and NSF-CBET 0609107

Monday, March 10, 2008 8:00AM - 11:00AM – Session A40 DCMP: Phase Stability and Phase Transitions Morial Convention Center 232
8:00AM A40.00001 First-principles solution to the problem of Mo lattice stability. IGOR ABRIKOSOV, CHRISTIAN ASKER, ARKADY MIKHAYLYUSHKIN, Department of Physics, Chemistry and Biology, Linköping University, Sweden — The energy differences between the ground state body-centred structure (bcc) and closed-packed face-centred structure (fcc) structures for transition metals in the middle of the series show unusually large disagreements when they are obtained by the thermochemical approach based on the analysis of experimental data or by first-principles electronic structure calculations. Considering a typical example, the lattice stability of Mo, we present a solution to this long-standing problem. In contrast to conventional total energy calculations within Density Functional Theory framework, we carry out ab initio molecular dynamics simulations for the two phases at high temperature. We show that at these conditions the fcc structures of Mo are dynamically stable, and the difference in their configurational energies decreases dramatically as compared to the zero temperature result, approaching the value derived by means of the thermochemical approach. We show that the main contribution to the effect comes from the modification of the canonical band structure for bcc and fcc phases due to lattice vibrations at high temperature, and discuss consequences of our finding for future first-principles simulations of phase stability.

8:12AM A40.00002 Link between structural and mechanical stability of fcc- and bcc-based ordered Mg-Li alloys. MAJE PHASHA, Materials Science and Manufacturing, CSIR, Pretoria, SA, PHUTI NGOEPE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, HASANI CHAUKE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, DUC NGUYEN-MANH, UKEA, Culham Science Centre, Oxfordshire, UK, DAVID PETTIFOR, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK — The first principles pseudopotential calculations based on the Perdew-Burke-Ernzerhof (PBE) form of generalized gradient approximation (GGA) within density functional theory (DFT) have been used to successfully investigate the electronic and elastic properties of cubic-based Mg-Li alloys. The heats of formation, Jones-type analysis and mechanical elasticity were utilized in predicting structural stability profile, and their results consistent with each other. An interesting correlation between shear modulus (C11) and the predicted energy differences of corresponding bcc and fcc ordered compounds relative to hcp Mg and Li lattices is observed.

8:24AM A40.00003 Density-Functional and CALPHAD Studies of U-Zr Alloys. ALEXANDER LANDA, PER SODERLING, PATRICE TURCHI, Lawrence Livermore National Laboratory, Livermore, CA 94551, USA, LEVENTE VITOS, ANDREI RUBAN, Royal Institute of Technology, Stockholm, SE-10044, Sweden — The U-Zr alloy alloys have been recognized as a fuel for liquid-metal fast breeder reactors. First-principles methods are employed to study ground-state properties of U-Zr alloys for the most important phases observed experimentally, namely γ (bcc) and δ (C32). Effective interatomic interactions obtained from the screened GPM, incorporating KKR-ASA-CPA, have been applied in MC simulations to derive the γ-δ miscibility gap. EMTO-CPA method has been applied to study properties of the open κ-phase. Results of ab initio calculations are compared with experimental data and CALPHAD assessment. Then, the CALPHAD assessed U-Zr phase diagram is contrasted with the one predicted with the input from ab initio. This work shows that an overall validity of a combined ab initio—CALPHAD approach to thermodynamic properties exists, and that the knowledge and quantitative output gained from quantum mechanics on phase stability and its relation to f-bonding, can be used to explore other actinide-based systems, for which experimental data are sparse or lacking. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

8:36AM A40.00004 Phase Stability Studies of Ni3Al and Pt3Al Structures. HASANI CHAUKE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, RALF DRAUTZ, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK, BENOIT MINISINI, ISMANS, 44 Avenue Bartholdi, 72000 Le Mans, FRANCE, PHUTI NGOEPE, Materials Modeling Centre, University of Limpopo, SOVENGA, SA, DAVID PETTIFOR, Materials Modeling Laboratory, Department of Materials, University of Oxford, Oxford, UK — The structural instability of cubic L12 against the non-cubic DO′C and tP16 Pt3Al have been investigated in direct comparison with Ni3Al, using plane-wave pseudopotential methods within the local density approximation. We predict that the deleterious DO′C is more stable than cubic ductile L12 Pt3Al, in agreement with the experimental observation of the LT DO′C phase and HT L12 phase. In contrast to the Pt-Al, the L12 Ni3Al is ground state and is consistent with the experimental phase diagram. The transformation from L12 into DO′C has been investigated more explicitly, where the transformation path along DO′C leads to a stable phase at displacement parameter u=0.0417. However the Ni3Al phase, is stable at u=0.0 corresponding to the cubic L12 phase, as expected. The phonon dispersion spectra have been used to confirm the relative structural trend where a soft mode was detected for L12 and DO′C which is not found in tP16 Pt3Al.

8:48AM A40.00005 Where are Nature’s missing structures1. GUS L.W. HART, Brigham Young University — Our society’s environmental and economic progress depends on the development of high-performance materials such as lightweight alloys, high-energy-density battery materials, recyclable motor vehicle and building components, and energy-efficient lighting. Meeting these needs requires us to understand the central role of crystal structure in a material’s properties. Despite more than 50 years of progress in first-principles calculations, it is still impossible in most materials to infer ground-state properties purely from a knowledge of their atomic components—a situation described as ‘scandalous’ in the well-known essay by Maddox. Although the key to the generic nature of the approach is energy minimization, the extrema are found in a chemistry-independent way.

1Supported by NSF DMR-0650406.

9:00AM A40.00006 Fully ab initio melting curve of aluminium up to 350 GPa. JOHANN BOUCHET, FRANCOIS BOTTIN, GERALD JOMARD, Commissariat à l’Energie Atomique — We performed ab initio molecular dynamics simulations to compute the melting curve of aluminium. Both the two-phase (TP) and heat-until melt (HUM) methods have been considered. The former describes an heterogeneous mechanism with a well-defined melting temperature Tm. On the other hand, in the HUM the crystal melts homogeneously and can be overheated above Tm. The limit of superheating is the critical temperature Te. Calculations are carried out in the NVT ensemble up to 350 GPa with supercells of different sizes. For each method, we present the convergence of the melting curves as a function of the number of atoms, and compare our results with previous calculations and experiments. We also discuss the evolution of the degree of overheating with respect to the pressure. At last, by means of NPT simulations we also compute volume change on melting, which is in good agreement with previous free energy calculations.

9:12AM A40.00007 Free energies from ab initio calculations for liquid Mg. RAQUEL LIZARRAGA, Universidad Austral de Chile, CARL GREEFF, Los Alamos National Laboratory — We performed free energy calculations for liquid metals from ab initio potential surfaces by means of Monte Carlo methods that involve sampling on the potential surface defined by a reference system. This allows for large gains in efficiency because the random walk is carried out on the much faster reference potential, and the ab initio potential is only evaluated on a small subset of uncorrelated configurations. This is highly desirable since direct free energy calculations for liquid metals from ab initio potential surfaces are very computationally intensive. Our calculations on liquid magnesium show that we can obtain free energies accurate at the meV/atom level with only 100 evaluations of the ab initio total energies.
9:24AM A40.00008 Ultrafast melting and solidification of Ag studied by time-resolved third harmonic generation, WAI LUN CHAN, VIRGINIA MCCREARY, ALEXIE LAGOUTCHEV, University of Illinois, Urbana-Champaign, YINON ASHKENAZY, The Hebrew University of Jerusalem, KWANGU KANG, DAVID CAHILL, ROBERT AVERBACK, University of Illinois, Urbana-Champaign. — We study the transformation of Ag between the solid and liquid phases using pump-probe femtosecond laser experiments. A pump with fluences of 100-500 mJ cm⁻² is used to heat the sample while third harmonic generation of light from a time-delayed probe is used to determine the structure as a function of time. For the melting experiment, we find that the solid begins to melt before the phonons are thermalized by the electrons, according to the two-temperature model. In addition, we find by using Ag thin films with different thicknesses, that the depth of heat deposition is less than 100nm. Both observations suggest that the established two-temperature model is insufficient to explain the melting kinetics in Ag by the femto-second laser. For the solidification experiment, we are able to determine the solidification velocity as a function of undercooling down to half of the melting temperature. The results are compared to predictions from molecular dynamics simulations.

9:36AM A40.00009 Revisiting the segregation driving forces rule: the Coupled Three Effects Model, JÉRÔME CREUZE, ISABELLE BRAEMS, FABIENNE BERTHIER, LEMHE/ICMMO, UMR 8182, Universite Paris Sud-XI, Bat. 410, F91405 Orsay cedex, France., CHRISTINE MOTTET, GUY TRÉGLIA, CRMCN-CNRS, Campus de Luminy, Case 913, 13288 Marseille cedex 9, France., BERNARD LEGRAND, SRMP-DIMN, CEA Saclay, F91911 Gil-sur-Yvette cedex, France. — Separating the surface segregation enthalpy into three elementary contributions (cohesive, alloy and size) has been proposed by many authors, but rarely tested quantitatively. Such a separation rule, derived from a tight-binding Hamiltonian years ago, has yielded very satisfying results for various environments (surfaces, grain boundaries and clusters) for the Cu-Ag system and for many other alloys, but recently stumbled over the Co-Pt system. We propose a new approach based on a systematic study of the permutation enthalpies, both in the bulk and in the surface, as a function of the mixed interaction involved in the N-body interatomic potentials derived from the electronic structure. We then show that both the disagreement observed for Co-Pt and the agreement mentioned for Cu-Ag can be explained by the variation of the effective pair interactions in the surface and by the existence of coupling coefficients between the three effects. Finally, we introduce a new decomposition, the Coupled Three Effects Model (CTEM), that is valid for systems with both size and cohesive effects.

9:48AM A40.00010 Ambient-temperature Conditioning as a Probe of Double-C Transformation Mechanisms in Pu-2 at. % Ga.¹ JASON R. JEFFRIES, K.J.M. BLOBAUM, M.A. WALL, A.J. SCHWARTZ, Lawrence Livermore National Laboratory — The gallium-stabilized Pu-2.0 at. % Ga alloy undergoes a partial or incomplete low-temperature martensitic transformation from the metastable delta phase to the monoclinic alpha-prime phase near -120 °C. This transformation has been shown to occur isothermally and it displays anomalous double-C kinetics in a time-temperature-transformation diagram. While the underlying mechanisms responsible for the double-C behavior are currently unresolved, recent experiments suggest that a conditioning treatment influences the upper-C. As such, the effects of the conditioning treatment can provide valuable insight into the mechanisms dominating the phase transition. A differential scanning calorimeter (DSC) is used to investigate the effects of conditioning temperature and time upon the delta/alpha-prime transition. The results will be discussed as they pertain to radiation damage, nucleation, embryo formation, or phase-field stability.

¹This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:00AM A40.00011 New Transformation Path of Shape Memory NiTi¹, N. HATCHER, O. YU. KONTSEVOI, A.J. FREEMAN, Northwestern University — The detailed mechanism of structural evolution during the martensitic transformation in NiTi is not fully understood. To fully characterize the transformation path and to precisely determine the structure of its martensitic phase, we employ the highly-precise all-electron full-potential linearized augmented plane wave (FLAPW) method² and identify the governing processes of the martensitic transformations between the B2, B19, R, B19' and recently proposed B33 and BCO phases. Several precursor phenomena for displacive phase transformations in the B2, B19, and R phases are identified, i.e. soft C_{14} and C' elastic constants, regions of Fermi surface nesting, and instabilities towards electronic topological transitions. By means of generalized stacking fault calculations, we find that the B2 phase has a low resistance to (100)⟨110⟩ shear. A new, barrierless transformation path from B2 to B19' is established by calculating a bilayer (100)⟨110⟩ shear with full structural optimization which leads to a monoclinic intermediate phase at 1/2a displacement; a relaxation of this structure's monoclinic angle results in the B19' phase.

¹Supported by AFOSR (grant # FA9550-07-1-0174).

10:12AM A40.00012 Magneto-Resistance at the Pre-Martensite Transition in Ni₅MnGa, C. P. OPEIL, Boston College, J. C. LASHLEY, J. L. SMITH, Los Alamos National Laboratory — A magneto-resistance and angle resolved photoemission (ARPES) study of the pre-martensite phase of the ferromagnetic shape memory alloy single crystal Ni₅MnGa, reveals a temperature (235 > T > 190 K) and field dependent (0 – 1 T) positive/negative magneto-resistance slope. Previous inelastic neutron scattering experiments (Zheludev et al., PRB 51, 1995) on this Heusler alloy indicate a phonon branch [110]-TA₂ softening in the pre-martensite phase along q = (1/3, 1/3, 0). This phonon softening combine with our ARPES data that show significant depletion of states (pseudo gap) occur at the premartensitic transition temperature. Recent results (Shapiro et al., EPL 77, 2007) reveal phases associated with the charge density wave (CDW) resulting from Fermi surface (FS) nesting. Our experimental results will be discussed in light of electron-phonon coupling.

10:24AM A40.00013 Optical properties of ErH₂₊ₓ: First principles calculations and experimental measurements, CLARK SNOW, THOMAS MATTSSON, Sandia National Laboratories — Rare earth and transition metal hydrides exhibit many interesting physical phenomena, from metal-semiconductor transitions to transparency changes at RT as a function of hydrogen content. Electrical resistivity measurements by P. Vajda (1) indicate that ErH₂₊ₓ undergoes a metal-semiconductor transition between 240-290K and an antiferromagnetic transition between 1.75-2.3K depending on hydrogen content. These same transitions should also cause profound changes in the optical properties. This work will present first principles calculations of the optical properties of ErH₂₊ₓ from 300-600K where x ranges from -0.2 to 0.2. The calculations will be compared to experimental results on thin films of ErH₂₊ₓ which were obtained as a function of temperature from 10-600K and hydrogen content.

¹Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.
10:36 AM A40.00014 Role of defects and impurities on the thermal stability of transition-metal nitrides and carbides, L. TSETSERIS, N. KALFAGIANNIS, S. LOGOTHEITIDIS, Aristotle University of Thessaloniki, Thessaloniki, Greece, S. T. PANTELIDES, Vanderbilt University, Nashville, TN — Transition-metal nitrides and carbides are used in a variety of applications because of their renowned hardness and stability. Here, we present the results of first-principles calculations on point defects and impurities in the prototype systems of TiN and TiC, and in HfN and ZrN. We find features which are common to all systems, while we unravel also key differences. In cases, for example Ni interstitials in TiN, the interaction between defects is attractive and it favors the formation of defect complexes. Moreover, we show that the atomic-scale mechanisms of interaction and migration of point defects and their complexes can account for various changes of transition metal nitrides and carbides after annealing at widely different temperatures. Finally, we discuss the fundamentals of trapping and release of the most common impurities in TiN. The work was supported in part by the McMinn Endowment at Vanderbilt University, AFOSR MURI Grant FA9550-05-1-0306, and GSR-PTENED-03ED613.

10:48 AM A40.00015 Atom Transport in Random Close Packed Metal Alloys under Thermal Forcing, YONG W. KIM, Lehigh University — Alloy making entails disparate pyro-metallurgical pathways, contributing to variability in elemental composition profiles. Surface segregation by constituent elements is a long-standing example. Thermal cycling and exposures to intense fluxes of energetic particles and photons, as in fission and fusion reactors, force the movement of composition profiles. Transport properties thus become dependent of materials’ history. We note that a non-crystalline alloy specimen is a randomly close packed assembly of atoms, and, as such, contains a distribution of residual nano-crystallites. The primary effect of varied forcing mechanisms is to convert atoms bound in nano-crystallites into those of glassy configurations. Spatial fluctuation is increased, specific to elemental species. In this paper we present a modeling of thermal conversion of crystallite atoms into a glassy state. The distribution function of nano-crystallites by size at room temperature is modeled by the distribution of nano-clusters formed from an atomic vapor plume. [Kim, Lee, Belony, Rev. Sci. Instr. 17, 10F115 (2006)] At a given temperature, equilibrium dissociation of a nano-crystallite into ‘glassy’ atoms is treated by the law of mass action. The equation of state is fashioned after the thermal expansion of the specimen volume with respect to a reference. A large set of simultaneous dissociation equations is solved iteratively. Work supported in part by NSF-DMR(Metals).

Monday, March 10, 2008 11:15AM - 2:15PM – Session B1 DCMP: Strongly Correlated Electrons in One Dimension Morial Convention Center LaLouisiane AB

11:15AM B1.00001 Narrow-gap Luttinger liquid in carbon nanotubes, LEONID LEVITOV, MIT — Single-walled carbon nanotubes are the thinnest and the cleanest among the currently available nanoscale quantum wires. Transport properties of nanotubes depend on the presence of a gap in electron spectrum, defining two main nanotube types, metallic and semiconducting. Semiconducting tubes attract interest in particular because of the sensitivity of their properties to external fields and doping. Among semiconducting tubes there is an interesting class of narrow-gap tubes, or so-called chiral metallic tubes, which exhibit a narrow semiconducting gap arising due to curvature [1]. The Luttinger liquid effects, which are strong in all nanotubes, are particularly interesting in the narrow-gap tubes. Interaction strongly affects the energy gap, reinforcing it and making it sensitive to the long-wavelength charge mode dynamics [2]. We discuss new types of charge carriers possible in the gapped states and their relation to recent experimental work [3].


11:51AM B1.00002 Observation of spin-charge separation and localization in one-dimensional quantum wires1, OPHIR AUSLAENDER2, Stanford University — We have been able to measure hallmark properties of electrons confined to one-dimensional (1D) wires. Profoundly affected by interactions, the 1D electron liquid is a Luttinger-liquid. Single particle elementary excitations, which survive in spite of interactions in higher dimensions, completely lose their integrity in a Luttinger-liquid. Instead, the elementary excitations of the 1D electron liquid are all collective, with long range correlations and are spin-charge separated. In spite of the drastic influence of electron-electron interactions on the many-body states, the observation of these effects in experiment has been elusive. Our wires were fabricated from a GaAs/AlGaAs heterostructure using cleaved edge overgrowth. The sample I shall discuss contained two parallel wires, 20nm and 30nm thick, which were separated by a 6nm insulating AlGaAs barrier. A series of top gates allowed us to contact each wire separately, and thus allowed us to control both the energy and the momentum of the electrons tunneling between the wires. The resulting tunneling conductance was a direct measure of the spectral function in each of the wires, and thus enabled us to map the dispersions of the 1D many-body elementary excitations. Pushing the wires to low density allowed us to probe the regime where interactions dominate over kinetic energy. In this regime we clearly observed two spin modes and one charge mode of the coupled wires. Mapping the dispersion velocities as a function of decreasing density, we found good agreement between the data and theoretical calculations of the velocity of the antisymmetric charge mode of the coupled wires. The theory also predicted an additional symmetric charge mode, that was not observed. The spin velocities were found, within experimental precision, to be smaller than theoretically predicted. Reducing the density of electrons even further, we found an abrupt transition in the extent of the 1D states along the wires: At high densities they were extended and had well defined momenta, while at low densities they localized as a result of interactions and exhibited Coulomb blockade physics. A simultaneous measurement of the two-terminal conductance, which displayed the typical stepwise drop with decreasing density, showed that a localization transition was concurrent with each conductance drop.

1Experiments performed at the Weizmann Institute of Science.
2In collaboration with H. Steinberg, A. Yacoby, Y. Tserkovnyak, B. I. Halperin, K. W. Baldwin, L. N. Pfeiffer, and K. W. West.

12:27PM B1.00003 The One-Dimensional Wigner Crystal in Carbon Nanotubes1, VIKRAM DESHPANDE, Applied Physics, Caltech — Electron-electron interactions strongly affect the behavior of low-dimensional systems. In one dimension (1D), arbitrarily weak interactions qualitatively alter the ground state producing a Luttinger liquid (LL) which has now been observed in a number of experimental systems. Interactions are even more important at low carrier density, and in the limit when the long-ranged Coulomb potential is the dominant energy scale, the electron liquid is expected to become a periodically ordered solid known as the Wigner crystal. In 1D, the Wigner crystal has been predicted to exhibit novel spin and magnetic properties not present in an ordinary LL. However, despite recent progress in coupled quantum wires, unambiguous experimental demonstration of this state has not been possible due to the role of disorder. We propose using low-temperature single-electron transport spectroscopy that a hole gas in low-disorder carbon nanotubes with a band gap is a realization of the 1D Wigner crystal [1]. We observe for the first time three distinct regimes as a function of carrier density and axial magnetic field: (I) a completely spin and isospin polarized state, (II) an isospin polarized, spin antiferromagnetic state, and (III) an unpolarized state with a four-fold addition energy period. The transitions among these regimes can be quantitatively and intuitively explained using a Wigner crystal picture based on a gapped LL model [2] with the carriers represented by spatially localized solitons. Our observation provides a clean platform for testing theories of interacting electrons in 1D and also indicates the possibility of using this many-body state for solid-state quantum information processing. [1] V. V. Deshpande and M. Bockrath, arXiv:0710.0683
[1] With Prof. Marc Bockrath (Applied Physics, Caltech)
1:03PM B1.00004 Fermi-Edge Singularity in a Spin-Incoherent Luttinger Liquid, GREGORY A. FIETE, University of Texas at Austin — In recent years the spin-incoherent Luttinger liquid, obtained in the energy window \( E_{\text{pin}} \ll k_B T \ll E_{\text{charge}} \), has attracted much attention because of its qualitatively distinct properties relative to the more familiar Luttinger liquid \[1\]. Some of the most remarkable effects appear in correlations in which the number of particles is abruptly changed, such as single particle Green’s function \[2\] or in the Fermi-edge singularity when a particle-hole pair is photo-excited \[3\]. In this talk, I draw on the methods developed in Ref.\[2\] to study the Fermi-edge singularity in the spin-incoherent Luttinger liquid \[3\]. Both cases of finite and infinite core hole are explored, as well as the effect of a static external magnetic field of arbitrary strength.

For a finite mass core hole the absorption edge behaves as \( (\omega - \omega_{\text{th}})^{3/2} / \sqrt{\ln(\omega - \omega_{\text{th}})} \) for frequencies \( \omega \) just above the threshold frequency \( \omega_{\text{th}} \). The exponent \( \alpha \) depends on the interaction parameter \( K_c \) of the excited one dimensional system, the electron-hole coupling, and is independent of the magnetic field strength, the momentum, and the mass of the excited core hole (in contrast to the spin-coherent case). In the infinite mass limit, the spin-incoherent problem can be mapped onto an equivalent problem in a spinless Luttinger liquid for which the logarithmic factor is absent, and backscattering from the core hole leads to a universal contribution to the exponent \( \alpha \).


1:39PM B1.00005 Transition from a one-dimensional to a quasi-one-dimensional state in interacting quantum wires\[1\], KONSTANTIN MATVEEV, Argonne National Laboratory — At low density, all electrons in a quantum wire occupy the lowest state of transverse quantization, and it is natural to view the system as one-dimensional. As the density is increased, the electrons start to populate the second subband, resulting in a transition to a quasi-one-dimensional state. I will discuss this transition in the presence of electron-electron interactions in a model that neglects electron spins. Clearly, in the non-interacting case the transition is accompanied by the emergence of a second gapless excitation mode. On the other hand, at very strong interactions, the one-dimensional electrons form a Wigner crystal, and the transition corresponds to it splitting into two chains. Unlike the non-interacting electrons, this two-row (zigzag) crystal still has only one acoustic excitation branch. This raises the question of how the nature of the transition to a quasi-one-dimensional state changes with interaction strength. We can show that in the vicinity of the transition already arbitrarily weak interactions open a gap in the second excitation mode. We then argue that only one gapless mode exists near the transition at any interaction strength.

\[1\] This work was supported by the U.S. Dept. of Energy, Office of Science, under contract DE-AC02-06CH11357.

Monday, March 10, 2008 11:15AM - 1:39PM –
Session B2 GMAG: Magnetism in Semiconductors: New Frontiers
Morial Convention Center LaLouisiane C

11:15AM B2.00001 Optical Properties of III-Mn-V Ferromagnetic Semiconductors, KENNETH BURCH, Los Alamos National Laboratory — We discuss the important role optical studies have played in our understanding of the electronic structure of III-Mn-V ferromagnetic semiconductors. These extensive studies have established the electronic structure is strongly affected by the strength of the exchange between the Mn local moments and the holes they introduce. Particular focus is given to Ga\textsubscript{1-x}Mn\textsubscript{x}As, where spectroscopic studies suggest the metallic state is unconventional. Finally, we will detail our recent experiments into the ultrafast manipulation of magnetism on the nanoscale. This work is in collaboration with D.B. Shrekenhamer, E.J. Singley, D.N. Basov (University of California, San Diego) J. Stephens, S. Mack, R.K. Wakamaki, D.D. Awschalom(University of California, Santa Barbara), B.L. Sheu, N. Samarth (Pennsylvania State University), F. Chen, A. Azad, J. O’Hara, A.M. Dattelbaum, G. Montano, S. Crooker, and A.J. Taylor (Los Alamos National Laboratory).

11:51AM B2.00002 Spin Transport in Ferromagnet-Semiconductor Heterostructures\[1\], PAUL CROWELL, University of Minnesota — Over the last two years, there has been significant progress in the integration of metallic ferromagnets with semiconductors, resulting in devices in which spin-polarized carriers are injected and detected electronically. I will discuss experiments on epitaxial Fe/GaAs Schottky tunnel barrier heterostructures patterned into lateral devices in which the ferromagnetic injection and detection contacts are separated by several microns.\[1\] The Schottky barrier consists of a highly-doped n\textsuperscript{+} region \( (n^+ \approx 5 \times 10^{18} \text{ cm}^{-3}) \) and the channel of the device is n-doped GaAs \( (n \approx 2 \times 10^{16} \text{ cm}^{-3}) \). A non-equilibrium spin polarization generated by electrical injection is detected potentiometrically using the non-local transport technique applied originally to metallic systems. An important aspect of this approach is the observation of spin precession and dephasing in the semiconductor channel (the Hanle effect), allowing for electrical measurements of the spin lifetime and diffusion length. We find a strong non-linear dependence of the spin polarization on the injection voltage, which we have investigated by preparing samples with different thicknesses of the channel of the device and varying the tunnel barrier profile. We find a systematic change in the spin accumulation observed under forward and reverse bias currents as the thickness of the n\textsuperscript{+} region increases. Other aspects of these devices have also been explored. For GaAs channels that are doped near the metal-insulator transition, the non-equilibrium electron spin polarization leads to dynamic nuclear polarization, which has a profound impact on the electron spin dynamics at low temperatures. Finally, I will discuss some important considerations for applications in which a bias current flows in the detector. [1] X. Lou et al., Nature Physics 3, 197 (2007)

\[1\] In collaboration with X. Lou, C. Adelmann, E.S. Garlid, Q. Hu, T. Kondo, J. Zhang, S.D. Flexner, K.S.M. Reddy, S.A. Crooker, and C.J. Palmstrom and supported by ONR, the NSF MRSEC, NNI, and IGERT programs, and the Los Alamos LDRD program.

12:27PM B2.00003 Ultrafast Photoinduced Non-thermal Phenomena in (III, Mn)V Ferromagnetic Semiconductors, JIGANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory — Magnetic materials display carrier-mediated exchange interaction are ideal for non-thermal, potentially fast spin manipulation and detection. Prominent examples of such materials are Mn doped III-V semiconductors such as GaMnAs, in which the strong interaction of carriers (holes) and Mn ions results in high transition temperature ferromagnetism. The steady-state magneto-optical/transport measurements reveal rich magnetic memory effects and strong enhancement of ferromagnetism via external stimuli (i.e., light, electrical field or current). However, no time-resolved experiments in (III,Mn)V semiconductors have shown these collective magnetic phenomena, and hence their time scales are completely unknown. In this talk, I will present our recent observations in GaMnAs of: (1) ultrafast enhancement of ferromagnetism via photoexcited transient holes on a 100 ps time scale and (2) femtosecond detection of magnetic memory states. Our measurements reveal new fundamental collective magnetic processes at ultrafast time scales, and identify the critical roles of the Mn-hole correlation in these photo-induced cooperative behaviors. These results constitute the first evidence for ultrafast, non-thermal manipulation of the spin order in (III,Mn)Vs, which may represent as-yet-undiscovered universal features in all carrier-mediated ferromagnetic materials.
1:03PM B2.00004 Ferromagnetism and localization in Ga$_{1-x}$Mn$_x$As, Ga$_{1-x}$Mn$_x$P, and in between$^1$, OSCAR DUBON, U.C. Berkeley and Lawrence Berkeley National Laboratory — Because of their potential as both injectors and filters of spin-polarized carriers, ferromagnetic semiconductors may play an important role in spin-based electronics, or spintronic devices. Ferromagnetic semiconductors are formed by the substitution of a relatively small fraction of host atoms with a magnetic species. Ga$_{1-x}$Mn$_x$As has been the most thoroughly studied material among these, and ferromagnetism in it arises from hole-mediated inter-Mn exchange. The Curie temperature $T_C$ in Ga$_{1-x}$Mn$_x$As has been shown to increase with increasing concentration of substitutional Mn acceptors. However, room temperature ferromagnetism in this canonical system has been elusive due to challenges in materials synthesis—namely, raising $x$ while avoiding the formation of second phases or compensating defects. Increasing $p-d$ exchange by modifying the host semiconductor via anion substitution (e.g., replacing As with P) is a significantly less explored route by which $T_C$ may be raised. We are investigating the effect of anion substitution in ferromagnetic Ga$_{1-x}$Mn$_x$As$_1-y$P$_y$ formed by ion implantation followed by pulsed-laser melting. In the endpoint compound Ga$_{1-x}$Mn$_x$P $T_C$ is found to vary linearly with $x$, and non-metallic transport is observed for $x$ up to $\sim$4.2%, corresponding to a $T_C$ of $\sim$62 K compared to $\sim$112 K for Ga$_{1-x}$Mn$_x$As with a similar $x$. Dilution of the endpoint compound Ga$_{1-x}$Mn$_x$As with P results in a precipitous decrease in $T_C$ to below 60 K for $y=2.8\%$. Remarkably, Ga$_{1-x}$Mn$_x$As$_1-y$P$_y$ films undergo a metal-insulator transition between $y=1.5\%$ and 2.3% even as $x$ is held approximately constant indicating that alloy disorder in the anion sublattice induces hole localization, which in turn may be responsible for a strong suppression of $T_C$. Thus, while anion substitution may enhance $p-d$ exchange, localization effects must be considered when developing a suitable picture for ferromagnetism in these materials.

$^1$Supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

Monday, March 10, 2008 11:15AM - 2:15PM – Session B3 FIAP: Silicon Photonics Morial Convention Center RO2 - RO3

11:15AM B3.00001 Silicon lasers, integration, interconnect, etc. at Intel , MARIO PANICCIA, Director Photonics Technology Lab, Intel Corporation — In this talk, we discuss integrated silicon photonics technologies that enable Tbit/s optical link for future VLSI interconnect applications. We also review the recent advances in various fundamental building blocks, including high-speed silicon optical modulator, SiGe detector, and hybrid silicon laser.

11:51AM B3.00002 Ultrafast Silicon Photonics Modulators , MICHAL LIPSON, Cornell University — No abstract available.

12:27PM B3.00003 Silicon integrated nanophotonics for on-chip interconnects$^1$, YURI VLASOV, IBM — Current trend in microelectronics industry is to increase the parallelism in computation by multi-threading, by building large scale multi-chip systems and, more recently, by increasing the number of cores on a single chip. With such increase of parallelization the interconnect bandwidth between the racks, chips or different cores is becoming a limiting factor for the design of high performance computer systems. The on-chip ultrahigh-bandwidth silicon-based photonic network might provide an attractive solution to this bandwidth bottleneck. We will review recent results on silicon nanophotonic circuits based on photonic wires and photonic crystals. Strong light confinement at the diffraction limit enables dramatic scaling of the device area and allows unprecedented control over optical signals. Silicon nanophotonic devices have immense capacity for low-loss, high-bandwidth data processing that might enable the design of ultra-compact on-chip optical networks. In particular we will show recent results on design and characterization of various ultra-compact (<0.03mm$^2$) silicon nanophotonic circuits as optical delay lines, electro-optic modulators, broadband optical switches, wavelength filters, etc.

$^1$Yuriy A. Vlasov, Fengnian Xia, William Green, Solomon Assefa

1:03PM B3.00004 Silicon Detectors, Sensors and Ultrafast Interconnect. , MEHDI ASGHARI, Kotura — No abstract available.

1:39PM B3.00005 Monolithic Integration of Photonic and Electronic Circuits in a CMOS Process , ATTILA MEKIS, Luxtera — We present our approach to a low-cost, highly scalable opto-electronic integration platform in silicon. We have developed a process in a commercial CMOS foundry that enables tightly integrated photonic devices and electronic circuits. The device library includes optical and opto-electronic components as well as electronic circuits. In this talk, we detail the performance of the building blocks and highlight the performance trade-offs encountered in integrating different functions on the same chip. We describe an opto-electronic circuit design toolkit, which is modeled after the standard electronic design flow and builds on commercial circuit design tools. The design flow includes automated design rule checking and layout-versus-schematic checks covering all types of circuit elements. As an example, we detail the design of a multi-channel transceiver chip with 10 Gbps/channel optical data transmission speed and report on its performance.


11:15AM B4.00001 Stimuli Responsive Vesicles, Micelles and Rods from Polypeptide-based Block Copolymers , DANIEL SAVIN, University of Vermont — The self-assembly of amphiphilic block copolymers is dictated primarily by the balance between the hydrophobic core volume and the hydrophilic corona. In these studies, amphiphilic block copolymers containing poly(lysinine) (P(Lys)) blocks were synthesized and their solution properties studied using dynamic light scattering, circular dichroism spectroscopy and transmission electron microscopy. The hydrophobic block used was either poly(2-butene) or a statistical copolymer of propylene oxide and ethylene oxide. The latter polymer exhibits a tunable critical point, below which the block copolymer is in the “double hydrophilic” limit. In these multiply-responsive materials, we exploit secondary structure changes that occur within the P(Lys) chain to observe changes in solution morphology as a function of solution conditions. At high pH, the P(Lys) chain assumes either an $\alpha$-helical or $\beta$-sheet conformation depending on temperature, while at lower pH the side chains become protonated, resulting in an expanded coil configuration. The effect of morphology changes due to these structural transitions will be discussed in the context of the interfacial curvature changes with $\text{pH}$ and temperature. These dynamic materials have potential applications as viscosity modifiers, liquid crystals and gels.
11:51AM B4.00002 Templated Self Assembly of Block Copolymer Thin Films, ALAMGIR KARIM. PPARC/NERC, University of Manchester and University of Essex — We study the shearinduced assembly of block copolymers in the early stages of development, providing insights into the fundamental behavior of these materials. The process involves the self-assembly of well-ordered periodic structures at a length scale of 10-100 nm. We explore the generality of this curvature cancellation phenomenon.

12:27PM B4.00003 Single Molecules and Surface Induced Nanopattern in Ultrathin Block-copolymer Films - Scanning Force Microscopy, MARA IOS, University of Manchester and University of Essex — We study the self-assembly of block copolymers in the early stages of development, providing insights into the fundamental behavior of these materials. The process involves the self-assembly of well-ordered periodic structures at a length scale of 10-100 nm. We explore the generality of this curvature cancellation phenomenon.

1:03PM B4.00004 Using block copolymer assembly to tailor surface properties, CHRISTOPHER OBER, The University of Texas at Austin — We study the self-assembly of block copolymers in the early stages of development, providing insights into the fundamental behavior of these materials. The process involves the self-assembly of well-ordered periodic structures at a length scale of 10-100 nm. We explore the generality of this curvature cancellation phenomenon.

1:39PM B4.00005 Integration of block copolymers into lithographic processes, PAUL NEALEY, University of Wisconsin — We study the self-assembly of block copolymers in the early stages of development, providing insights into the fundamental behavior of these materials. The process involves the self-assembly of well-ordered periodic structures at a length scale of 10-100 nm. We explore the generality of this curvature cancellation phenomenon.

Monday, March 10, 2008 11:15AM - 2:15PM — Session B5 DCMP: Geometry and Elasticity, Morial Convention Center R01

11:15AM B5.00001 Generalized Crumpling: induced singularities in gently deformed elastic sheets, THOMAS WITTMAN, University of Chicago — If a thin disk of elastic material is confined in a shrinking sphere, the deformation of the disk is not smooth but nearly singular when its radius becomes larger than that of the sphere: the curvature at a point diverges as the thickness goes to zero. This talk considers induced singularities that arise from the interaction of these "vertex" singularities with their environment. For example, if two vertices are present, the curvature on the line joining them also diverges, forming the familiar ridge singularity [1]. Other induced singularities are coming to light. Here we consider two such singularities. The first is the induced vertex at the boundary [2] of a disk that has been compressed until it contains two interior vertices. Asymptotically, the triangular region bounded by the three vertices becomes arbitrarily flat as the sheet thickness goes to zero, while the curvature outside approaches a nonzero limit. The second singularity appears when a vertex is formed by forcing a flat sheet into a circular ring so that the sheet buckles. Then the ring force induces a singular radial curvature in the sheet. Remarkably this curvature just sufficient to make the mean curvature vanish where the ring contacts the sheet [3].

We explore the generality of this curvature cancellation phenomenon.

1 T. A. Witten, Rev. Mod. Phys. 79 643 (2007)

11:51AM B5.00002 Columnar and crystalline monolayers on curved substrates, VINCENZO VITELLI, University of Pennsylvania — We study thin self-assembled columns constrained to lie on a curved, rigid substrate. The curvature presents no local obstruction to equally spaced columns in contrast to curved crystals for which the crystalline bonds are frustrated. Instead, the vanishing compressional strain of the columns implies that their normals lie on geodesics which converge (diverge) in regions of positive (negative) Gaussian curvature, in analogy to the focussing of light rays by a lens. The bending of the layers generates a pre-stress of geometric frustration in the ground state that exists prior to the inclusion of defects. This simple observation is the basis for a versatile analytical approach to calculate the geometrical forces between dislocations and Gaussian curvature in columnar as well as in crystalline monolayers. The resulting forces play an important role in stress relaxation dynamics, elastic instabilities, and melting.

1We gratefully acknowledge the NSF/UW NSEC and the Semiconductor Research Corporation for funding.

1Penn MRSEC Grant DMR-0520020
12:27PM B5.00003 The shape, stability and dynamics of elastic surfaces. L. MAHADEVAN, Harvard University — Bending a thin sheet is easier than stretching it, an observation which has its roots in geometry. We will use this fact to explain some unusual problems in biology, physics and geology. At the everyday scale, I will discuss the morphology of avascular algal blades, the dynamics of defects in an elastic ribbon, and the dynamics of prey capture by certain carnivorous plants. At the geological scale, I will try to explain the shape of island arcs on our planet. Finally, time permitting, I will discuss how we might extend these ideas to the macromolecular scale, to derive a mechanical model for the dynamic instability of a growing microtubule.

1:03PM B5.00004 Elasticity and capillarity: wet hairs and origami. BENOIT ROMAN1, PMMH - Paris — Capillary forces are responsible for a large range of everyday observations: the shape of rain droplets, the imbibition of a sponge, the clumping of wet hair into bundles. Although they are often negligible on macroscopic structures, surface capillary forces may overcome volume forces at small scales and deform compliant micro-structures. Capillary-induced sticking can indeed prevent the actuation of mobile elements in micro-electro-mechanical systems (MEMS), or even cause their collapse. Capillary forces also have important consequences in biology such as the buckling of the airway lumen induced by surface tension, which can eventually cause the lethal closure of lung airways (known as neonatal respiratory distress syndrome). We will review a few experimental situations where capillary forces are able to deform two types of objects: rods, and thin sheets. For instance, the nanotubes of a “carbon nanotube carpet” self-assemble into conical “teepee” structures after the evaporation of a solvent and can produce intriguing cellular patterns. Similarly, macroscopic wet hairs tend to assemble into bundles through a cascade of successive pairings. Comparing attracting capillary forces to bending elasticity, leads to a characteristic “elasto-capillary” length. The case of thin sheets is challenging because of geometrical constraints, which generally leads to singularities. Can a thin sheet spontaneously wrap around droplet? We will describe in detail this “capillary origami” experiment.

1 together with José Bico

1:39PM B5.00005 Folding and swirling instabilities of viscous fluid threads in microchannels. THOMAS MASON1, Depts. of Physics and Chemistry, University of California-Los Angeles — We study the behavior of viscous fluid threads formed by hydrodynamic focusing as they are swept along by the flow of a different outer fluid in hard microfluidic channels. By examining pairs of miscible liquids for which interfacial tension is essentially absent, such as silicone oils having different molecular weights, we reveal a rich variety of fluid instabilities that occur at low Reynolds numbers. When a single thread that propagates stably in the center of a straight channel encounters a divergence in the channel’s width, the thread simply dilates if its viscosity is similar to that of the outer fluid. However, due to the extensional flow and deceleration in the diverging channel, a thread that is sufficiently viscous becomes unstable and reduces energy dissipation by performing sinusous bending oscillations, or ‘folding’, rather than dilating. By tuning the flow rates, we reveal a novel period-doubling route to chaotic folding. The folding and stretching of a thread in a diverging channel provides a simple means of mixing viscous liquids and creating controlled viscosity gradients. Moreover, using a sequence of two cross-channels, we make a pair of viscous threads that become unstable when swept along near the walls of a straight channel as a result of the viscous torque induced by the velocity gradient. The amplification of lateral undulations ultimately causes the threads to break up and form an array of viscous swirls, the miscible counterpart of droplets. This swirling instability provides a means for producing discrete and uniform ephemeral swirls, the miscible counterpart of droplets. By injecting three different miscible liquids into a dual cross-channel geometry, we examine the complex patterns that form when several fluid instabilities interact and compete. Overall, we anticipate that these measurements will provide important insight into the behavior of flowing threads in which interfacial tension plays a more substantial role.

In collaboration with: T. Cubaud.

Monday, March 10, 2008 11:15AM - 2:15PM
Session B6 GQI DAMOP: Quantum Simulation and Quantum Information Theory in Cold Atoms Morial Convention Center R04

11:15AM B6.00001 Cold atoms in 1D. ULRICH SCHOLLWOECK, RWTH Aachen — Ultracold atoms in optical lattices present a wealth of phenomena in one-dimensional geometries. In this talk, I will focus on specifically one-dimensional phenomena such as spin-charge separation in fermionic systems and the bosonic counterpart, as well as models of collective magnetism realized in ultracold atom systems. Special emphasis will be given to the observation of coherent quantum dynamics far from equilibrium which we can now simulate using the time-dependent density-matrix renormalization group method, in order to use cold atoms to address questions of relaxation to steady states in interacting quantum systems.

11:51AM B6.00002 Probing Phase Transitions in Cold Atoms1. ANATOLI POLKOVNIKOV, Boston University — In this talk I will describe various interferometric probes, which can be used to study correlation functions of low-dimensional cold atom systems. These probes allow one to analyze both properties of phases with long or quasi-long range order and phase transitions. I will suggest the way of detecting fermionic superfluidity and the symmetry of the pairing gap. I will also discuss connections between interferometry in 1D bosonic systems with partition functions of some condensed matter models and with extreme value statistics. Finally I will describe the shot noise and argue how one can suppress it both for bosons and fermions using optical lattices.

1Supported by AFSOR YIP

12:27PM B6.00003 Quantum Control with Ultracold Atoms1. IVAN DEUTSCH, University of New Mexico — Ultracold atoms have long been considered as a platform for quantum information processing. Of critical importance is the ability to coherently control both internal degrees of freedom such as spin and also interactions between atoms that depend on “external” motional degrees of freedom. In this talk I will review a variety of advances, including the ability to perform qudit operations such as state preparation and unitary gates, quantum-state reconstruction via continuous measurement, and cooling of atomic motion without decohering spin qubits. Two different platforms will be presented — alkali atoms transported in a lattice with microwave-induced spin-flips, and alkaline-earth atoms in which quantum information is stored in nuclear spins. Microwave-induced spin flips provide a robust mechanism for inducing cold collisions between atoms that can form the basis of a quantum logic gate. As an alternative, cold alkaline-earth atoms are attractive since the ground state is a closed shell, with zero electron angular momentum. The nuclear spin is thus decoupled from the system and can acts as robust decoherence-free qubit.

1Supported by NSF, ONR, DTO.
1:03PM B6.00004 Imaging single atoms in a three dimensional array1. DAVID WEISS, Penn State — We have demonstrated trapping and imaging of 250 single atoms in a 3D optical lattice. The 5 micron lattice spacing is large enough that individual atoms can be addressed using lasers and microwaves in a way that does not affect the quantum coherence of other atoms. Our goal is to use these trapped atoms as qubits. So far, we fill a random half of the lattice sites, but a combination of site-selective state changes and state-selective lattice translations should allow us to verifiably fill all vacancies. We will describe our experiments to date and our plans for entangling atoms and implementing a neutral atom quantum computer. Our lattice can readily be scaled to include thousands of trapped atoms. This work was performed in collaboration with Karl Nelson and Xiao Li.

1This work was supported by the Army Research Office

1:39PM B6.00005 Atomtronics. MURRAY HOLLAND, University of Colorado at Boulder — We explore the analogy between ultracold atoms in optical lattices and electrons in crystal lattices. Of particular interest is atomtronics, where the analogy is extended to include electrical circuits and doped semiconductor materials. Lattice “defects” achieve behaviors similar to P-type and N-type semiconductor materials. Naturally the interest is to adjoin P-type and N-type atoms lattices to produce an atom diode, and then an NPN or PNP lattice “sandwich” to achieve bipolar transistor-like behavior for ultracold atoms.

Monday, March 10, 2008 11:15AM - 2:15PM — Session B7 DBP GSNP: Gene Regulation Morial Convention Center R05

11:15AM B7.00001 Max Delbruck Biological Physics Prize Talk: The Biophysics of Gene Regulation, Studied One Molecule at a Time1. STEVEN BLOCK2, Stanford University — Advances have led to a new field, dubbed single molecule biophysics. Prominent among the new technologies is the optical trap, or ‘optical tweezers.’ Sensitive systems for measuring force and displacement in optical traps permit the nanomechanical properties of individual macromolecules to be explored with unprecedented precision, revealing behaviors heretofore obscured by ensemble-based approaches. This talk will focus on some of our current work with single-molecule systems, including transcription by RNA polymerase and structural transitions in nucleic acids. We developed high-resolution instrumentation that has broken the nanometer barrier and is thereby able to detect displacements down to the atomic level, in aqueous buffer at room temperature. Consequently, we can monitor the motions of RNA polymerase molecules in real time as these step from base to base along DNA. On the practical side, base-pair resolution makes it possible to sequence DNA in a new way, based on enzyme motions, and points to new directions in nanoscience. The improved stability afforded by the current generation of optical trapping apparatus has allowed us to reconstruct the complete energy landscapes for folding transitions in nucleic-acid hairpins. Recently, we have turned our attention to the problem of co-transcriptional folding, aptamers, and riboswitches formed in nascent mRNAs, and to the DNA or RNA sequence elements that regulate expression.

1research supported by the NIGMS
2Delbruck Prize Lecture

11:51AM B7.00002 Using DNA mechanics to predict intrinsic and extrinsic nucleosome positioning signals1. ALEXANDRE MOROZOV, Rutgers University — In eukaryotic genomes, nucleosomes function to compact DNA and to regulate access to it both by simple physical occlusion and by providing the substrate for numerous covalent epigenetic tags. While nucleosome positions in vitro are determined by sequence alone, in vivo competition with other DNA-binding factors and action of chromatin remodeling enzymes play a role that needs to be quantified. We developed a biophysical, DNA mechanics-based model for the sequence dependence of DNA binding energies, and validated it against a collection of in vitro free energies of nucleosome formation and a nucleosome crystal structure; we also successfully designed both strong and poor histone binding sequences ab initio. For in vivo data from S.cerevisiae, the strongest positioning signal came from the competition with other factors rather than intrinsic nucleosome sequence preferences. Based on sequence alone, our model predicts that functional transcription factor binding sites tend to be covered by nucleosomes, yet are uncovered in vivo because functional sites cluster within a single nucleosome footprint and thus make transcription factors bind cooperatively. Similarly a weak enhancement of nucleosome binding in the TATA region becomes a strong depletion when the TATA-binding protein is included, in quantitative agreement with experiment. Our model distinguishes multiple ways in which genomice sequence influences nucleosome positions, and thus provides alternative explanations for several genome-wide experimental findings. In the future our approach will be used to rationally alter gene expression levels in model systems through redesign of nucleosome occupancy profiles.

1Supported by the Lehman Brothers Foundation through a Leukemia and Lymphoma Society fellowship

12:27PM B7.00003 Towards a Quantitative Understanding of Single-Gene Transcription. DÁIBHID Ó MAOLÉIDIGH1. Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — The transcription of the genetic information in DNA into RNA is the first step in protein synthesis. This process is highly regulated and is carried out by RNA polymerase (RNAP), a complex molecular motor. Here we discuss some of the consequences of a Brownian ratchet model of transcription, which incorporates internal structural degrees of freedom of RNAP and kinetic barriers to backtracking of RNAP resulting from steric clashes with co-transcriptionally folded RNA. This approach was previously used (a) to successfully predict sequence dependent positions of pauses during the elongation process [1,2]; (b) to study the behavior of a number of mutants of RNAP, with different elongation behaviors, believed to involve different internal motions of the enzyme [3]; and (c) to gain insight into the interpretation of single-molecule transcription elongation experiments [2]. The same model can be used to characterize the stability of the elongation complex at specific termination sequences, places along DNA where, with high probability, RNAP releases the RNA transcript and disengages from the template. Recent experimental results on termination reinforce a picture of the elongation complex as a flexible structure, not a rigid body [4]. In more general terms, some of the modeling to be presented raises fundamental issues related to “model comparison” and “model selection,” the problem of identifying and characterizing quantitative models on the basis of limited sets of experimental data [5].

1This work was supported by the Army Research Office


[1]In collaboration with: Andrei E. Ruckenstein, Office of the Provost, Boston University; Vasisht R. Tadigota, Dept. of Physics, Boston University; Evgeny Nucler, Dept. of Biochemistry, New York University Medical Center.
1:03PM B7.00004 Information flow and optimization in transcriptional regulation. GASPER TKACIK, Princeton University — In the simplest view of transcriptional regulation, the expression of a gene is turned on or off by the changes in the concentration of a transcription factor (TF). Here we analyze transcriptional regulatory elements with the tools of information theory. Recent data on noise levels in gene expression are used to show that it should be possible to transmit much more than just one regulatory bit. Realizing this optimal information capacity would require that the dynamic range of TF concentrations used by the cell, the input/output relation of the regulatory module, and the noise levels of binding and transcription satisfy certain matching relations. This parameter-free prediction is in good agreement with recent experiments on the Bicoid/Hunchback system in the early Drosophila embryo, and this system achieves around 90% of its theoretical maximum information transmission. The dependence of information capacity on parameters that govern gene expression for simple, single-input / single-output, genetic regulatory elements is systematically examined and the extensions of the work to genetic circuits consisting of several interacting elements are presented.

1:39PM B7.00005 The Genomic Code for Nucleosome Positioning, JONATHAN WIDOM, Dept. of Biochemistry, Molecular Biology and Cell Biology, and Dept. of Chemistry, Northwestern University — Eukaryotic genomes encode an additional layer of genetic information, superimposed on top of the regulatory and coding information, that controls the organization of the genomic DNA into arrays of nucleosomes. We have developed a partial ability to read this nucleosome positioning code and predict the in vivo locations of nucleosomes. Our results suggest that genomes utilize the nucleosome positioning code to facilitate specific chromosome functions including to delineate functional versus nonfunctional binding sites for key gene regulatory proteins, and to define the next higher level of chromosome structure itself.

Monday, March 10, 2008 11:15AM - 2:15PM – Session B8 DFD: Colloidal Self-Assembly II Morial Convention Center R06

11:15AM B8.00001 Orthogonal Tracking Microscopy for Nanofabrication Research. MATTHEW MCMAHON, ANDREW BERGLUND, PETER CARMICHAEL, JABEZ MCCLELLAND, J. ALEXANDER LIDDLE, National Institute of Standards and Technology — Constructing two-dimensional lateral particle trajectories from digital video sequences of nanoparticle motion in a liquid is straightforward and fairly common, requiring only the use of centroid-finding algorithms. On the other hand, extracting particle trajectories in the third (out-of-plane) dimension has been more difficult, requiring detailed calibration of the radius of the defocused diffraction rings which result from vertical fluctuations of particle position. We introduce a new technique, termed orthogonal tracking microscopy or orthogonal projection microscopy, in which integrated micromirrors produce one or more reflected images of a particle within the same field of view as the direct image. The reflected images project vertical motion into lateral motion. Thus, we are able to construct a fully 3D particle trajectory from 2D digital video using only centroid-finding algorithms. We use this technique to study particle-surface interactions relevant to directed assembly of nanoparticles.

11:27AM B8.00002 Self-Assembly of Colloidal Membranes, EDWARD BARRY, ZVONIMIR DOGIC, Brandeis University — Symmetric monolayer membranes are observed to self-assemble in a colloidal suspension of hard rods with soft attractions. This attractive component to the interaction is enough to drive the self-assembly of stable two dimensional fluid-like surfaces of rods. Simultaneous measurements are made at both the molecular, via direct imaging of individual fluorescently labeled particles, and the continuum length scales. At the continuum scale, the elastic Hamiltonian for a two dimensional fluid-like surface is verified for a symmetric monolayer, and measured material constants such as the bending modulus and the area compression modulus are demonstrated to obey a simple elastic relationship.

11:39AM B8.00003 Self-Assembled 3D Ordered Macroporous Structures for Tissue Engineering Scaffolds, WEN-TAU JUAN, KUO-YUAN CHUNG, Institute of Physics, Academia Sinica, Taipei, Taiwan, NARAYAN MISHRA, Dept. of Paper Technology, Indian Institute of Technology, Roorkee, KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan — A simple, inexpensive and fast microfluidic method to fabricate three-dimensional ordered macroporous gel is demonstrated using alginate as the scaffold material. The microfluidic device consists of two concentric micropipettes where one is nested inside the other. Nitrogen gas and aqueous alginate solution with Pluronic F127 are pumped through the inner and the outer channel respectively. Under appropriate conditions, bubbles of a uniform size are generated within the device at few thousand Hz. We show the control over bubble size by the gas pressure and quantitatively predict the size dependence from the geometry of fluidic device. Monodisperse bubbles are collected and self-assemble into crystal structures as wet foam. The alginate solution between bubbles is crosslinked by divalent calcium ions and turns into 3D ordered macroporous gel where the pores are highly interconnected. The pore size can be directly controlled by the bubble size which ranges from few tens microns to few millimeters. This technique promises a versatile and robust way to make 3D ordered tissue engineering scaffolds.

11:51AM B8.00004 Five-fold attractor in two-dimensional diffusion processes, GUILERMO RAMIREZ-SANTIAGO, Instituto de Física, UNAM, CARLOS I. MENDOZA, Instituto de Investigaciones en Materiales, UNAM — We introduce an algorithm to generate two-dimensional diffusion-limited star-branched polymers (DLSP) attaching monomers successively to a central colloidal particle with any desired number of reactive sites. The proposed algorithm produces star-shaped aggregates whose final structure at relatively large distances from the central colloid has five-fold symmetry independently of the initial number of reactive sites. Therefore, the final morphology can be considered as a universal attracting distribution for this irreversible diffusion-limited aggregation process.

1:03PM B8.00005 Template-Guided Langmuir-Blodgett Deposition of Colloidal Particles, JAEHYUN HUR, YOU-YEON WON, Purdue University — We present a new method of fabricating highly-ordered two-dimensional (2D) colloidal crystals with non-closed-packed symmetries. In this method, using the Langmuir-Blodgett (LB) monolayer deposition technique, we transfer a Langmuir monolayer of colloidal particles constructed at the air-water interface onto a substrate which contains micro-fabricated topological patterns. We demonstrate that by using this template-guided LB deposition method, a perfect single 2D colloidal crystal structure that is homogeneous throughout the entire area of the patterned substrate can be economically fabricated under appropriate LB processing conditions. We investigate the effects of various control parameters (such as the initial particle density at the air-water interface, the substrate lifting speed, and the humidity condition during the LB monolayer deposition) on the structural properties of the resultant LB colloidal monolayer. As the compression area or the lifting speed is increased, the average density of the deposited particles in the resultant LB colloidal monolayer becomes reduced. The evaporation of water causes an undulation in the deposited particle density profile along the substrate lifting direction. We present a theoretical model which can quantitatively explain all these experimental observations.

We acknowledge partial financial support by DGAPA-UNAM project IN-107607 and CONACYT 43596-F.

12:03PM B8.00006 Template-Guided Langmuir-Blodgett Deposition of Colloidal Particles, JAEHYUN HUR, YOU-YEON WON, Purdue University — We present a new method of fabricating highly-ordered two-dimensional (2D) colloidal crystals with non-closed-packed symmetries. In this method, using the Langmuir-Blodgett (LB) monolayer deposition technique, we transfer a Langmuir monolayer of colloidal particles constructed at the air-water interface onto a substrate which contains micro-fabricated topological patterns. We demonstrate that by using this template-guided LB deposition method, a perfect single 2D colloidal crystal structure that is homogeneous throughout the entire area of the patterned substrate can be economically fabricated under appropriate LB processing conditions. We investigate the effects of various control parameters (such as the initial particle density at the air-water interface, the substrate lifting speed, and the humidity condition during the LB monolayer deposition) on the structural properties of the resultant LB colloidal monolayer. As the compression area or the lifting speed is increased, the average density of the deposited particles in the resultant LB colloidal monolayer becomes reduced. The evaporation of water causes an undulation in the deposited particle density profile along the substrate lifting direction. We present a theoretical model which can quantitatively explain all these experimental observations.
12:15PM B8.00006 Clustering in Hard Core/Soft Shoulder Lattice Gas Models. Paul D. Beale, University of Colorado at Boulder. Charles A. Sievers, Matthew A. Glaser — Isotropic hard core/soft shoulder interacting particle models have been shown to display a wide variety of thermodynamic phases: structured liquids, micellar solids, layered and columnar liquid crystals, and a variety of modulated solid phases. We have explored the phase diagram of a class of lattice gas models that are designed to approximate continuum models. We use generalizations of Baxter’s hard hexagon model on a two-dimensional hexagonal lattice to model the hard core repulsions. The longer-ranged repulsive soft shoulder is included to induce a Klein/Likos clustering instability. The clustering instability creates softly interacting fluidic micelles, as well as several type of modulated solid phases. The lattice model allows the observation of two different solid phase models, typically only display liquid phases with short-range order and solids with long-range order that is commensurate with the underlying lattice. Preliminary results indicate the model exhibits soft solid phases composed of fluidic micelles that form a quasi-long ranged solid phase characteristic of continuum solid phases in two dimensions. We will also present a mean field theory analysis of the initial clustering instability.

12:27PM B8.00007 Elastic Theory of Defects in Toroidal Crystals. Luca Giomi, Mark Bowick, Syracuse University — Crystalline assemblages of identical sub-units packed together and elastically bent in the form of a torus have been found in the past ten years in a variety of systems of surprisingly different nature, such as viral capsids, self-assembled monolayers and carbon nanomaterials. We investigate the structural properties of toroidal crystals and we provide a unified description based on the elastic theory of defects in curved geometries.

12:39PM B8.00008 Two-dimensional hopping of aqueous colloidal clusters on commensurate surface wells. Minsu Kim, Physics, UIUC, Stephen Anthony, Chemistry, UIUC, Steve Granick, Material Science and Engineering, UIUC — Hopping of colloidal clusters in various shapes and sizes that are mainly confined within commensurate surface wells except for diffusing between them by Brownian motion is studied. The mobility of clusters decreases nonmonotonically with increasing cluster size. The mobility proceeds, depending on cluster shape, by different jumping mechanisms such as zigzagging or translation without rotation; this produces nonmonotonic changes of mobility when, at fixed cluster size, cluster shape varies. Unlike atomic clusters that change configuration and dissociate easily, these colloidal clusters are very stable and each type of jump can be identified separately. Hopping rate, diffusion and different jumping mechanisms that are associated with them will be discussed for various sizes and shapes of clusters.

12:51PM B8.00009 Complexity from Specificity: Light Scattering and Colloidal Studies of Dscam Self-Association. Jesse Collins, Harvard School of Engineering and Applied Science (SEAS), Natalie Arkus, Harvard SEAS, Guanganmeng, Harvard Physics, Michael Brenner, Harvard SEAS, Dietmar Schmucker, Dana Farber Cancer Institute, Vinothan Manoharan, Harvard SEAS and Department of Physics — The self-assembly of complex structures from nanometer-sized building blocks is of great technological importance (i.e., for the development of tissue scaffolds and photonic crystals) and is of significant basic scientific interest. Here I present light scattering and colloidal aggregation studies of Dscam, a protein with over 18,000 splice variants which all (or almost all) exhibit exclusively homophilic binding, and which is necessary for the generation of structural complexity in the brain of insects. Static and dynamic light scattering data reveal the statistical mechanical properties of Dscam self-association, including the free energy, second virial coefficient, and oligomer molecular weight. Finally, I demonstrate how to exploit Dscam’s unprecedented level of molecular diversity and specificity for the self-assembly of custom nano- and micro-structures out of Dscam-conjugated colloids.

1:03PM B8.00010 Non-spherical Depletants in Colloidal Suspensions. Stephen Barr, Erik Luijtjen, University of Illinois at Urbana-Champaign — We investigate the effective interactions between spherical colloids induced by rigid rod-like depletants. The size disparity between the colloids and the rods makes conventional simulation methods inefficient. We overcome this by extending the generalized geometric cluster algorithm for colloidal suspensions (J. Liu and E. Luijtjen, Phys. Rev. Lett. 92, 035504 (2004)) to systems of non-spherical particles. We investigate both uncharged and charged colloids and rods, where the electrostatic potential is modeled through a screened interaction. The dependence of the induced depletion potential on both the strength and the range of the electrostatic interactions is quantified. In case of a rod-shape depletion, the depletion attraction between the colloids is enhanced as the screening length becomes larger, owing to the increased effective size of the rods. Systems with a rod-shape attraction are also explored.

This work is supported by the National Science Foundation through Grant No. DMR-0346914.

1:15PM B8.00011 Magnetically assembled “ring-shaped” colloidal particle structures. Hui Son, Randall Erb, Duke University, Mechanical Engineering and Material Science, Bapappidya Samanta, Vincent Rotello, University of Massachusetts, Amherst, Chemistry, Benjamin Yellen, Duke University, Mechanical Engineering and Material Science — We demonstrate a convenient method for assembling ring-shaped colloidal structures by applying uniform magnetic field to a mixture of 2.7-μm paramagnetic beads, 1-μm non-magnetic polystyrene beads, and a fluid dispersion of 10-nm iron oxide nanoparticles (i.e., ferrofluid). The ferrofluid serves as a magnetic contrast medium and induces dipole moments in both the paramagnetic and non-magnetic beads when an external magnetic field is applied. We discovered that for certain volume fractions of ferrofluid, the attractive forces generated between the smaller non-magnetic beads and the larger magnetic beads induce the non-magnetic particles to form a ring structure around the circumference of the paramagnetic beads. This method differs from similar self-assembly techniques in that the ring structures form solely through magnetic force, rather than depending on random motion and patterned bonding.

1:27PM B8.00012 Effects of surface biotin density on lipid monolayer-assisted 2D crystallization of streptavidin at the aqueous solution-vapor interface. MasaFumi Fukuto, Matthew Loehr, Suntao Wang, Sumit KevalRamani, Lin Yang, Brookhaven National Laboratory — Adsorption and two-dimensional (2D) crystallization of soluble protein streptavidin on a biotinylated lipid monolayer at an aqueous solution-vapor interface have been studied extensively since the 1990s. These previous studies, largely based on fluorescence microscopy and ex-situ electron microscopy measurements, revealed the effects of protein modifications and aqueous buffer conditions, such as pH and ionic strength. We have examined the dependence of 2D streptavidin crystallization on the areal biotin density in the lipid monolayer template, using Brewster-angle microscopy (BAM) and in-situ x-ray reflectivity and grazing-incidence x-ray diffraction (GID). The lipid monolayer consisted of a binary mixture of DMPC and DPPE-x-biotin, and the biotin density was controlled by varying the lipid composition while keeping the area per lipid fixed. Both BAM and GID results demonstrate that in order for 2D crystallization of streptavidin to occur, the surface biotin density must exceed a threshold, corresponding to approximately two biotins per protein. The results highlight the importance of well-defined molecular orientations to the 2D crystallization of proteins.
Lipid Monolayers, Suntao Wang, Antonio Checco, Brookhaven National Laboratory, Zhongwei Niu, Qian Wang, University of South Carolina, Masafumi Fukuto, Lin Yang, Brookhaven National Laboratory — Bio-nanoparticles (large proteins, viruses) are ideal building blocks for creating ordered two-dimensional (2D) arrays. These 2D protein crystals or ordered arrays are of great scientific and technological interest. Here, we demonstrate the use of in-situ x-ray scattering and Brewster angle microscopy (BAM) to monitor the formation of self-assembled, 2D ordered arrays by tobacco mosaic viruses (TMVs) on a lipid layer that was either supported by a solid substrate or formed at the liquid-vapor interface. The lipid monolayer not only confines the viral particles within a plane, but also provided the lateral mobility that is crucial for developing structural order. In-situ X-ray scattering was used to provide real-time information on the structure of the virus array and guide optimizations of the surrounding chemical environment to improve in-plane structural order. The presence of Ca\(^{2+}\) ions is also essential to the formation of well-ordered, closely packed 2D arrays of TMV. Atomic Force Microscopy was also used to directly image the final structure to provide real space confirmation of developed structural order.

Non-equilibrium dynamics of virus capsid assembly, Artem Levandovsky, University of California Riverside — The process of self-assembly of nano-structures under non-equilibrium conditions has recently received a lot of attention in various fields. A viral shell (capsid) is, for one, one of the most interesting biological structures that can spontaneously form (from statistical mechanics point of view) at the right pH and ionic strength. While the viral capsids are by far less complex than most other biological objects, the process of virus assembly remains poorly understood. Viruses are found to adopt many different shapes. The mechanisms involved in the self-assembly of capsids into a particular shape as well as the transitions from spherical to non-spherical shells are the subject of this presentation. We show that the kinetic formation of the protein building blocks into the intermediate states (dimers, trimmers, pentamers and hexamers) can lead to the construction of shells with different morphologies.

Transportal thermal transport in colloidal silica system: effect of particle size and aggregation, Gang Chen, Fan Jiang, Department of Physics and Astronomy, Ohio University, Wenhua Yu, Jules Routbort, Energy Systems Division, Argonne National Laboratory, Department of Physics and Astronomy, Ohio University Team, Energy Systems Division, Argonne National Laboratory Collaboration — Knowledge of distribution of nanoparticles in solution is critical to understanding the observed enhancements of thermal conductivity in colloidal systems. We have applied small-angle x-ray scattering (SAXS) to study particle size and distribution of monodispersed and aggregated silica colloids. A hot-wire method has been used to measure thermal conductivity of the colloidal system. The results indicate that the thermal conductivity depends not only on the particle concentration, but also on the particle size and distribution. The experimental data contradict thermal transport models based on fluid interfacial layers or Brownian motion but shed light on the detrimental role of liquid-particle interface on the thermal transport properties.

Thermal conductivity in colloidal silica system: effect of particle size and aggregation, Gang Chen, Department of Physics and Astronomy, Ohio University, Wenhua Yu, Jules Routbort, Energy Systems Division, Argonne National Laboratory, Department of Physics and Astronomy, Ohio University Team, Energy Systems Division, Argonne National Laboratory Collaboration — Knowledge of the size and distribution of nanoparticles in solution is critical to understanding the observed enhancements of thermal conductivity in colloidal systems. We have applied small-angle x-ray scattering (SAXS) to study particle size and distribution of monodispersed and aggregated silica colloids. A hot-wire method has been used to measure thermal conductivity of the colloidal system. The results indicate that the thermal conductivity depends not only on the particle concentration, but also on the particle size and distribution. The experimental data contradict thermal transport models based on fluid interfacial layers or Brownian motion but shed light on the detrimental role of liquid-particle interface on the thermal transport properties.

Monday, March 10, 2008 11:15AM - 2:03PM — Session B9 GSNP: Pattern Formation and Nonlinear Dynamics Morial Convention Center R07

11:15AM B9.00001 Intermediate State in Type-I Superconducting Strip with Current1, Jacob Hoberg, Rulshan Prozorov, Iowa State University — The dynamic structure of the intermediate state was studied in pinning-free Pb strips using real-time magneto-optical visualization. It is found that topological hysteresis can be lifted by applying sufficiently large current. Namely, laminar structure that appears on flux exit in a static case is turned into tubular when the current is present. Temperature, magnetic field and current phase diagram is discussed.

1Supported by the DOE-BES contract No. DE-AC02-07CH11358, NSF grant No. DMR-05-53285 and Alfred P. Sloan Foundation.

11:27AM B9.00002 Generation of dynamic self-propelled structures by symmetry breaking mechanism in driven magnetic layers on the surface of liquid, Alexey Snezhko, Maxim Belkin, Igor Aranson, Argonne National Laboratory — Magnetic particles suspended over the surface of a liquid and energized by a vertical alternating magnetic field give rise to remarkable dynamic multi-segment magnetic structures (‘snakes’). These structures (dynamic by nature) are directly related to wave surfaces in the liquid generated by the collective response of magnetic microparticles to the alternating magnetic field. The self-assembly process and existence of the magnetic snakes is accompanied by a generation of strong surface flows in the liquid. Properties of the snake and corresponding surface flows could be tuned by the parameters of the external magnetic driving. We demonstrate that above some critical frequency threshold magnetic snakes lose their stability and start to swim in the container. The effect is attributed to the development of symmetry breaking instability of the structure with respect to self-generated surface flows in the liquid. Parameters of the driving magnetic field are effectively used to control rich behavior of the dynamic magnetic swimmers.

11:39AM B9.00003 Collective dynamics and pattern formation in 2D regular arrays of spherical particles in Stokes flow between two parallel walls1, Jerzy Blawzdziewicz, Yale University, Eligiusz Wajnryb, IPPT Warsaw, Poland, Matthew Baron, Nidhi Khurana, Yale University — We present results of our numerical and theoretical investigations of collective dynamics of linear trains and regular square arrays of spherical particles suspended in a fluid bounded by two parallel walls. The simulations reveal propagation of particle-displacement waves, deformation and rearrangements of a particle lattice, propagation of dislocation-like defects in ordered arrays, and transitions between ordered and disordered regions that can coexist for a long time. We argue that ordered motion of the arrays is associated with the dipolar form of the external magnetic driving. We demonstrate that above some critical frequency threshold magnetic snakes lose their stability and start to swim in the container. The effect is attributed to the development of symmetry breaking instability of the structure with respect to self-generated surface flows in the liquid. Parameters of the driving magnetic field are effectively used to control rich behavior of the dynamic magnetic swimmers.

1Work supported by NSF CAREER grant CTS-0348175

11:51AM B9.00004 Theory of slope-dependent disjoining pressure with application to Lennard-Jones liquid films, Taeil Yi, Harris Wong, Louisiana State University — A liquid film of thickness h < 100 nm is subject to additional intermolecular forces, which are collectively called disjoining pressure P. Since dominates at small film thicknesses, it determines the stability and wettability of thin films. Current theory derived for uniform films gives P=P(h). This solution has been applied recently to non-uniform films and becomes unbounded near a contact line as h→0. Consequently, many different effects have been considered to eliminate or circumvent this singularity. We present a mean-field theory of that depends on the slope as well as the height h of the film.[1] When this theory is implemented for Lennard-Jones liquid films, the new P=P(h,hu) is bounded near a contact line as h→0. Thus, the singularity in P(h) is artificial because it results from extending a theory beyond its range of validity. We also show that the new can capture all three regimes of drop behavior (complete wetting, partial wetting, and pseudo partial wetting) without altering the signs of the long and short-range interactions. We find that a drop with an unbounded precursor film is linearly stable.[1] Wu & Wong, J. Fluid Mech, 506, 157 (2004)2 Yi & Wong, J. Colloid Inter. Sci. 313, 579 (2007)
12:03PM B9.00005 The effects of chaotic mixing on patterns and fronts in an advection-reaction-diffusion system\footnote{Supported by NSF Grants DMR-0404961, DMR-0703635 and PHY-0552790.}, TOM SOLOMON, JEFFREY BOEHMER, Bucknell University — We present experimental studies of the effects of fluid flows on reaction fronts and spatial patterns in the excitable Belousov-Zhabotinsky reaction. The flow is a square array of vortices, generated using magnetohydrodynamic techniques. Time-dependent forcing of the flow is achieved by displacing the fluid periodically in a circular manner relative to the vortex flow. Mixing of passive impurities in this flow is chaotic, with long-range transport that is typically diffusive (enhanced), although superdiffusion with Lévy flights is also possible. Reaction fronts in this flow show small-scale patterns that reflect the stable and unstable manifolds that characterize chaotic mixing in this flow. Even on a larger scale, front structure reflects the underlying anisotropy of the vortex lattice. In many cases, the front mode-locks to the external forcing, lining up with the vortex array in a self-extracting manner. Self-generating trigger waves are also found in this system, producing both spiral and target patterns similar to those found in reaction-diffusion systems.

12:15PM B9.00006 Spatial Forcing in Thermal Convection, GABRIEL SEIDEN, STEPHAN WEISS, EBERHARD BODENSCHATZ, Max Planck Institute for Dynamics and Self-Organization — An intrinsic characteristic of thermal convection is the preference of a particular wavenumber at onset. This fact renders experimental investigations of different important aspects, such as the exploration of phase space, difficult. The main tool employed to overcome this difficulty is spatial forcing, whereby, using external means, one forces a desired pattern and observes the evolution of the system thereafter. We present results on topologically and optically induced modulations of large aspect ratio isotropic (horizontal) and anisotropic (inclined layer) Rayleigh-Bénard convection. These include detailed bifurcation curves and phase diagrams for different forcing scenarios.

12:27PM B9.00007 Renormalization group method for predicting frequency clusters in a chain of nearest-neighbor Kuramoto oscillators, OLEG KOGAN, GIL REFAEL, MICHAEL CROSS, Caltech, JEFFREY ROGERS, Caltech, HRL, CALTECH CONDENSED MATTER TEAM — We develop a renormalization group (RG) method to predict frequency clusters and their statistical properties in a 1-dimensional chain of nearest-neighbor coupled Kuramoto oscillators. The intrinsic frequencies and couplings are random numbers chosen from a distribution. The method is designed to work in the regime of strong randomness, where the distribution of intrinsic frequencies and couplings has long tails. Two types of decimation steps are possible: elimination of oscillators with exceptionally large frequency and renormalization of two oscillators bonded by a very large coupling into a single one. Based on these steps, we perform a numerical RG calculation. The oscillators in the renormalized chain correspond to frequency clusters. We compare the RG results with those obtained directly from the numerical solution of the chain’s equations of motion.

12:39PM B9.00008 Pattern morphology and dynamical scaling in the Cahn Hilliard model\footnote{The authors thank the Ohio Supercomputer Center, Kenyon College, the Liquid Crystal Institute at Kent State University, and the NSF (grant DMS0440299) for their support.}, TIMOTHY SULLIVAN, PUSHKAR DAHAL, Department of Physics, Kenyon College, PETER PALFY-MUHORAY, Liquid Crystal Institute, Kent State University — Numerical simulations were carried out in two-dimensions of the dimensionless Cahn-Hilliard equation. Simulations were run for a factor of ten in time beyond previously reported results. The simulations also covered a broad range of values of the mean composition, $\langle \psi \rangle_0$. To determine the dynamical scaling exponent, $b$, an equation of the form $R_2(t) = at^b + c$ was fit to a measure of average domain size. In contrast to previous results, we found that $b$ varied substantially with $\langle \psi \rangle_0$. The largest deviation from the Lifshitz-Slyozov value of 1/3 occurred at $\langle \psi \rangle_0 = 0.15$, where $b = 0.221 \pm 0.04$. We used a measure of the non-uniformity of minority domains to show that for $\langle \psi \rangle_0 \leq 0.20$ the domain shapes are not scale invariant for times exceeding our simulation times. We also point out the possible existence of a phase boundary $\langle \psi \rangle_{0,c}$ that separates a phase with circular domains of minority component from a phase with non-circular minority component domains.

12:51PM B9.00009 Experimental Evidence for Mixed Reality States\footnote{This work is supported in part by the NSF grant DMS 03-25939 ITR.}, VADAS GINTAUTAS, ALFRED HUBLER, Center for Complex Systems Research, Department of Physics, University of Illinois at Urbana-Champaign — We present experimental data on the limiting behavior of an inter-reality system: a virtual pendulum with a bi-directional instantaneous coupling to its real-world counterpart [Gintautas & Hubler, Phys.Rev.E 75, 057201 (2007)]. The data show that if the physical parameters of the simplified virtual system are close to the parameters of the real system, there is a phase transition from an uncorrelated dual reality state to a mixed reality state in which the motion of the two pendulums is highly correlated. As virtual systems better approximate real ones, even weak couplings in inter-reality systems may induce sudden transitions to mixed reality states. This phenomenon may be typical for systems with instantaneous coupling and was recently featured on the tip sheet of the American Physical Society [http://www.aps.org/about/tipsheets/tip68.cfm]. We show that mixed reality states in physical systems are related to out-of-body experiences of humans in 3D-video feedback systems [H. H. Ehrsson, The Experimental Induction of Out-of-Body Experiences. Science 317, 1048 (2007)].

1:03PM B9.00010 Classical dynamics simulations with pattern formation by metallic spheres with induced electrostatic interactions, PETER FLECK, ALFRED HUBLER, Center for Complex Systems Research, University of Illinois at Urbana-Champaign — We study classical dynamics simulations of metallic spheres immersed in a highly viscous, but weakly conducting medium while exposed to the electrostatic field of external electrodes of various geometries. We represent the system’s charge dynamics by the spheres’ multipole moments and determine the phase boundaries of this line formation behavior in the sphere dynamics simulations. We find the phase diagram to be in good agreement with analytical predictions.

1:15PM B9.00011 Hopping Conduction and Bacteria: Transport Properties of Disordered Reaction-Diffusion Systems, ANDREW MISSEL, KARIN DAHMEN, University of Illinois, Urbana-Champaign — Reaction-diffusion (RD) systems are used to model everything from the formation of animal coat patterns to the spread of genes in a population to the seasonal variation of plankton density in the ocean. In all of these problems, disorder plays a large role, but determining its effects on transport properties in RD systems has been a challenge. We present here both analytical and numerical studies of a particular disordered RD system consisting of particles which are allowed to diffuse and compete for resources ($\lambda \rightarrow A$) with spatially homogeneous rates, reproduce ($A \rightarrow 2A$) in certain areas (“oases”), and die ($A \rightarrow 0$) everywhere else (the “desert”). In the low oasis density regime, transport is mediated through rare “hopping events” in which a small number of particles diffuse through the desert from one oasis to another; the situation is mathematically analogous to hopping conduction in doped semiconductors, and this analogy, along with some ideas from first passage percolation theory, allows us to make some quantitative predictions about the transport properties of the system on a large scale.
in the role lattice strain plays between the copper oxide planes. We have examined Bi$_2$EISAKI, ALESSANDRA LANZARA — Towards understanding the physics of the high-temperature superconducting cuprates, there has been growing interest if not impossible, to observe in material plasma.

plasma. Using wave-kinetic theory and Wigner formalism, we interpret the speckles of statistical light as quasi-particles which can interact via the nonlinearity.

FLEISCHER, Princeton University, Princeton, NJ 08544, USA — We consider the nonlinear propagation of partially-spatially-incoherent light as a photonic interaction. The simulations were done for a chosen value of electric dipole moment and for a set of temperatures. Chain formation is observed when the potential is dipolar as well as when both terms are included. However, our simulation shows some differences in the pattern formation of the chains.

Monday, March 10, 2008 11:15AM - 2:15PM –

11:15AM B10.00001 Revealing pseudogap physics using lanthanide substituted Bi$_2$Sr$_{1.6}$Ln$_0$_0.4CuO$_{6+δ}$, DANIEL GARCIA, University of California, Berkeley. JEFF GRAF, CHRIS JOZWIAK, SHUYUN ZHOU, HIROSHI EISAKI, ALESSANDRA LANZARA — Towards understanding the physics of the high-temperature superconducting cuprates, there has been growing interest in the role lattice strain plays between the copper oxide planes. We have examined Bi$_2$Sr$_{1.6}$Ln$_0$_0.4CuO$_{6+δ}$ (Ln=La, Nd, Eu, Bi) near optimal doping using angle resolved photoemission spectroscopy. The increasing radius mismatch of the substituted lanthanide, which monotonically decreases the superconducting $T_c$, appears to also affect the electronic properties of these system. The effect of strain on Fermi arcs, superconducting gap and pseudogap physics will be discussed.

11:27AM B10.00002 A Laser Based ARPES Study of the Nodal Region of the Cuprates1, J.D. RAMEAU, CMPMSD, Brookhaven National Laboratory / Stonybrook University, H.-B. YANG, G.D. GU, P.D. JOHNSON, CMPMSD, Brookhaven National Laboratory — A new laser based facility has been constructed at the NSLS for studies of strongly correlated electron systems. While recent studies of the nodal and near-nodal spectrum of the cuprates with low energy lasers appear to show good agreement with correlated energy, synchrotron based ARPES, several adverse effects of performing ARPES with lasers remain to be explored. Using the new facility we show that the combination of high emission angles and low energy laser kinetic energies has many implications for the accurate measurement of any linewidth or band dispersion. We show that this is particularly so for the nodal and near-nodal single particle spectrum of the cuprates. The results and implications of our studies for future laser based ARPES are analyzed and discussed.

11:39AM B10.00003 Evidence for pairing above $T_c$ from the electronic dispersion in the pseudogap phase of cuprates, A. KANIGEL, Technion, Haifa 32000, Israel, U. CHATTERJEE, University of Illinois at Chicago, Chicago, IL 60607, M. RANDERIA, The Ohio State University, Columbus, OH 43210, M.R. NORMAN, Argonne National Laboratory, Argonne, IL 60439, J.C. CAM-PUZANO, University of Illinois at Chicago, Chicago, IL 60607 — In the BCS paradigm for the superconducting state, electrons close to the Fermi level $E_F$ form Cooper pairs which condense into a zero center of mass momentum state. This results in a gap in the electronic excitation spectrum which is symmetrically centered about $E_F$. Above $T_c$, where the condensate is lost, the pairs dissociate, the energy gap collapses, and the the normal state Fermi surface appears. On the other hand, in the underdoped high temperature superconductors, instead of a complete Fermi surface above $T_c$, only disconnected Fermi arcs appear, separated by regions that still exhibit an energy (pseudogap). We show that in this pseudogap phase, the energy-momentum relation of electronic excitations near $E_F$ behaves like the dispersion of a normal metal on the Fermi arcs, but like that of a superconductor in the gapped regions. We argue that this dichotomy in the dispersion is hard to reconcile with a competing order parameter, but is consistent with pairing without condensation. Below $T_c$ the pairs condense and the electronic excitations, that were short-lived above $T_c$, become long-lived and exhibit a d-wave energy gap.

11:51AM B10.00004 Possible Explanation of the Fermi Arcs in Cuprates, based on a clustered superconducting state above $T_c$1, GONZALO ALVAREZ, Oak Ridge National Laboratory, ELBIO DAGOTTO, University of Tennessee and ORNL — A previously introduced Landau-Ginzburg model [1] to describe the competition between antiferromagnetism and d-wave superconductivity in the cuprates is here further investigated. The state above the critical temperature $T_c$ is made of superconducting (SC) clusters, with a nonzero amplitude of the SC order parameter but random phase factors, coexisting with antiferromagnetic(AF) regions. This state disappears above a higher temperature scale $T^*$. The LDOS of this state is in good agreement with recent STM experiments [2]. Our main result is that the angle-resolved photoemission spectrum of this SC-AF clustered state contains Fermi surface arcs in the region $T < T_c < T^*$, very similar to those observed experimentally [3]. Low energy states created at the interface between clusters are responsible for the arcs. [1] G. Alvarez et al., Phys. Rev. B 71, 014514 (2005). [2] K. K. Gomes et al., Nature 447, 569 (2007). [3] A. Kanigel et al., cond-mat/0708.4099 (2007).

11:39AM B10.00003 Evidence for pairing above $T_c$ from the electronic dispersion in the pseudogap phase of cuprates. A. KANIGEL, Technion, Haifa 32000, Israel, U. CHATTERJEE, University of Illinois at Chicago, Chicago, IL 60607, M. RANDERIA, The Ohio State University, Columbus, OH 42210, M.R. NORMAN, Argonne National Laboratory, Argonne, IL 60439, J.C. CAM-PUZANO, University of Illinois at Chicago, Chicago, IL 60607 — In the BCS paradigm for the superconducting state, electrons close to the Fermi level $E_F$ form Cooper pairs which condense into a zero center of mass momentum state. This results in a gap in the electronic excitation spectrum which is symmetrically centered about $E_F$. Above $T_c$, where the condensate is lost, the pairs dissociate, the energy gap collapses, and the the normal state Fermi surface appears. On the other hand, in the underdoped high temperature superconductors, instead of a complete Fermi surface above $T_c$, only disconnected Fermi arcs appear, separated by regions that still exhibit an energy (pseudogap). We show that in this pseudogap phase, the energy-momentum relation of electronic excitations near $E_F$ behaves like the dispersion of a normal metal on the Fermi arcs, but like that of a superconductor in the gapped regions. We argue that this dichotomy in the dispersion is hard to reconcile with a competing order parameter, but is consistent with pairing without condensation. Below $T_c$ the pairs condense and the electronic excitations, that were short-lived above $T_c$, become long-lived and exhibit a d-wave energy gap.

11:51AM B10.00004 Possible Explanation of the Fermi Arcs in Cuprates, based on a clustered superconducting state above $T_c$1, GONZALO ALVAREZ, Oak Ridge National Laboratory, ELBIO DAGOTTO, University of Tennessee and ORNL — A previously introduced Landau-Ginzburg model [1] to describe the competition between antiferromagnetism and d-wave superconductivity in the cuprates is here further investigated. The state above the critical temperature $T_c$ is made of superconducting (SC) clusters, with a nonzero amplitude of the SC order parameter but random phase factors, coexisting with antiferromagnetic(AF) regions. This state disappears above a higher temperature scale $T^*$. The LDOS of this state is in good agreement with recent STM experiments [2]. Our main result is that the angle-resolved photoemission spectrum of this SC-AF clustered state contains Fermi surface arcs in the region $T < T_c < T^*$, very similar to those observed experimentally [3]. Low energy states created at the interface between clusters are responsible for the arcs. [1] G. Alvarez et al., Phys. Rev. B 71, 014514 (2005). [2] K. K. Gomes et al., Nature 447, 569 (2007). [3] A. Kanigel et al., cond-mat/0708.4099 (2007).

11:27AM B10.00002 A Laser Based ARPES Study of the Nodal Region of the Cuprates1, J.D. RAMEAU, CMPMSD, Brookhaven National Laboratory / Stonybrook University, H.-B. YANG, G.D. GU, P.D. JOHNSON, CMPMSD, Brookhaven National Laboratory — A new laser based facility has been constructed at the NSLS for studies of strongly correlated electron systems. While recent studies of the nodal and near-nodal spectrum of the cuprates with low energy lasers appear to show good agreement with correlated energy, synchrotron based ARPES, several adverse effects of performing ARPES with lasers remain to be explored. Using the new facility we show that the combination of high emission angles and low energy laser kinetic energies has many implications for the accurate measurement of any linewidth or band dispersion. We show that this is particularly so for the nodal and near-nodal single particle spectrum of the cuprates. The results and implications of our studies for future laser based ARPES are analyzed and discussed.

1This work is supported by the Department of Energy under Contract No. DE-AC02-98CH10886
12:03PM B10.00005 Understanding the Protected Nodes and the Fermi Arcs in the Cuprate Superconductors. QUIN CHEN, K. LEVIN, University of Chicago — We address a recent analysis of photoemission data which elucidates the superconducting phase of the underdoped cuprates. We first present a simple phenomenological approach to the spectral function which shows how the $d$-wave order parameter symmetry results in protected nodes, which, above $T_c$, broaden into Fermi arcs; this “protection” is associated with superconducting coherence rather than reduced thermal broadening. A microscopic theory, consistent with this phenomenology, is presented. It reconciles the observations that the excitation gap below $T_c$ is temperature independent while the superfluid density necessarily vanishes at $T_c$. Reference: Q.J. Chen, K. Levin, and I. Kosztin, Phys. Rev. B 63, 164519 (2001).

This work was supported by NSF Grants No. PHY-0555325 and No. MRSEC DMR-0213745.

12:15PM B10.00006 Pseudogap correlations inside the superconducting dome. ELENA BASCONES, BELEN VALENZUELA, Instituto de Ciencias Materiales de Madrid (CSIC) — Recent experiments[1,2] have uncovered, two energy scales, an antinodal energy $g_{an}$ and a nodal one in the superconducting phase of underdoped hole doped cuprates. This finding reminds the nodal-antinodal dichotomy seen in the pseudogap state. The competing Yang-Rice-Zhang[3] scenario for the pseudogap has shown to be useful to understand these experiments[4]. Here we explore the effect of the competition between pseudogap and superconductivity on the condensation energy and superfluid density which show deviations from the standard BCS behavior. We compare the theoretical results with experiments.


12:27PM B10.00007 Pseudogap and Superconducting Gap - Same or Different? W.S. LEE, J.M. VISHIK, K. TANAKA, R. MOORE, D.H. LU, T. SASAGAWA, Stanford University, N. NAGAOSA, T.P. DEVEREAUX, University of Waterloo, Z. HUSSAIN, ALS, National Lawrence Berkeley Lab, Z.X. SHEN, Stanford University — The pseudogap state in underdoped cuprates has been one of the central questions in high-$T_c$ research. Recently, whether pseudogap and superconducting gap are same energy gap or two different energy scales is strongly debated in data interpretation of single-particle spectrum, such as ARPES and STM. To gain further insight into this issue, detailed doping dependence and temperature dependence of the gap were studied using ARPES. In contrast to the behavior of the well-known pseudogap in the antinodal region, we found that the behavior of the gap is qualitatively different near the nodal region, a momentum space region overlooked in the previous measurements. This gap seems closely related to the superconductivity; it opens up at $T_c$ and reduces with decreasing doping in the deeply underdoped region following the trend of the superconducting dome in the heavily underdoped region of the phase diagram. The emerging two-gap phenomenon points to a picture of richer quantum configurations in high-$T_c$ superconductors.

This work is supported by DOE Office of Science, Division of Materials Science, with contract DE-FG03-01ER45929-A001 and NSF grant DMR-0604701.

12:39PM B10.00008 Different temperature evolution of electronic states in superconducting state and normal state in underdoped Bi2212 high-Tc superconductor , KIYOSHISA TANAKA, W.S. LEE, Stanford University, D.H. LU, Stanford Synchrotron Radiation Laboratory, R. MOORE, T. SASAGAWA, Stanford University, Z. HUSSAIN, Lawrence Berkeley National Laboratory, Z.X. SHEN, Stanford University — One of the most mysterious issues in high-Tc superconductor is an energy gap called “pseudogap”, well above $T_c$, which exists over a wide region of compositions and temperatures. The origin of this pseudogap and its relation to the superconducting gap are believed to hold the key for understanding the mechanism of high-Tc superconductivity. Recent angle-resolved photoemission spectroscopy (ARPES) revealed the coexistence of two distinct energy gaps in heavily underdoped samples which have opposite doping dependence [1]. One gap can be assigned as pseudogap and the other gap as superconducting gap because of the positive correlation between the gap magnitude and $T_c$. This result suggests that pseudogap arises from another mechanism and gives profound implications on the mechanism of high-Tc superconductivity. More recently, this two gap feature has been observed in the temperature dependence even in near optimally doped samples [2]. Detailed temperature dependence of ARPES spectra will be shown and the special character of pseudogap state will be discussed. [1] K. Tanaka et al., Science, 314, 1910 (2006). [2] W.S. Lee et al., Nature, 450, 81 (2007).

12:51PM B10.00009 Temperature and doping dependent ARPES study of the gaps in Bi2212. H.-B. YANG, CMPMSD, Brookhaven National Laboratory, J.D. RAMEAU, CMPMSD, Brookhaven National Laboratory / Stonybrook University, P.D. JOHNSON, T. VALLA, G.D. GU, A.T. TSVELIK, CMPMSD, Brookhaven National Laboratory, CMPMSD, BROOKHAVEN NATIONAL LABORATORY TEAM — High-resolution angle-resolved photoemission (ARPES) is used to probe the development of the gaps around the Fermi surface in Bi2212. A new method of data analysis is presented to remove the complications associated with the experimental resolution. Normalizing by the Fermi function then allows the observation of both the occupied and unoccupied states. The results on the temperature and doping dependence of the gap show that the underdoped system in the normal state behaves differently from all region of the phase diagram in the superconducting state, and point to potentially different origins for the pseudogap.

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

1:03PM B10.00010 Fermi arcs and phase diagram of the high- $T_c$ cuprates: Insights from Raman and angle resolved photoemission spectroscopies. JAMES STOREY, Victoria University of Wellington, JEFFERY TALLON, GRANT WILLIAMS, MacDiarmid Institute for Advanced Materials and Nanotechnology — We calculate the $B_{1g}$ and $B_{2g}$ Raman responses of Bi2212 from an ARPES-derived energy momentum dispersion and a model for the normal-state pseudogap. In light of these calculations, the Raman data demonstrates that the Fermi arc length remains finite in the pseudogap ground state. A re-examination of recent ARPES results is found to confirm this result. In addition, the presence of a van Hove singularity in the overdoped regime, as revealed by ARPES, allows us to propose a universal pairing potential that reproduces both the doping dependence of $T_c$ as well as the variation in $T_{c,\text{max}}$ between different species of cuprate superconductors.

1:15PM B10.00011 Hall Effect Signature of Fermi Surface Reconstruction in High- $T_c$ Superconductors. F.F. BALAKIREV, J.B. BETTS, A. MIGLIORI, Los Alamos National Laboratory, I. TSUKADA, Central Research Institute of Electric Power Industry, Japan, YOICHI ANDO, Osaka University, Japan, G.S. BOEBINGER, National High Magnetic Field Laboratory and Florida State University — The doping dependence of the Hall number in the normal state of two different HTS systems, La$_{2-x}$Sr$_x$CuO$_4$ and Bi$_{2-x}$Sr$_2$La$_x$CuO$_{6+\delta}$, exhibits an anomalous peak at optimum doping that emerges only at low temperatures. With increasing hole doping, as the pseudogap energy scale decreases, the peak onset is ascribed to the emergence of electron-like Fermi pockets in the Brillouin zone. The destruction of the peak beyond optimum doping suggests the destruction of the electron pockets and emergence of a large hole pocket, two phenomena that would result simultaneously with the loss of the Brillouin zone folding associated with the pseudogap state. The low temperature Hall resistance thus elucidates the Fermi surface evolution in the HTS cuprates, characterized by a zero temperature phase transition upon collapse of the pseudogap near optimum doping.

1This work was supported by the National High Magnetic Field Laboratory and the National Science Foundation.

2This work is supported by DOE Office of Science.
1:27PM B10.00012 Energy gaps in failed superconductor \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) - R.-H. HE. Dept of Phys, Appl Phys, SSRL, Stanford Univ., K. TANAKA, SSRL, Stanford and ALS, LBNL, S.-K. MO, SSRL, Stanford and ALS, Berkeley, T. SAGAWA, SSRL, Stanford and Mat. and Struct. Lab, TIT, Japan, M. FUJITA, Inst. of Mat. Res., Tohoku Univ, Japan, N. MANIELLA, SSRL, Stanford and ALS, Berkeley; K. YAMADA, Tohoku, Japan, Z. HUSSAIN, ALS, Berkeley, Z. SHEN. SSRU, Stanford — By angle-resolved photoemission spectroscopy with improved energy and momentum resolution, we find in the normal state of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \times = 1/8 \) a strong existence of the nodal quasi-particle together with a \( d \)-wave energy gap along the underlying Fermi surface extending over a significant range in the momentum space before an abrupt take-off of the gap close to the antinodal region. This suggests the presence of a novel nodal metal state, which is different from the one proposed that assumes a single \( d \)-wave extension of the pseudogap from the antinode toward the node along the whole underlying Fermi surface. This state is compatible with the static stripe ordering but only involves a precursor pairing of the electrons away from the antinodal region. We argue that the traditional pseudogap defined exclusively for the antinodal states has a distinct origin than its new nodal counterpart, i.e., a \( c \)-wave gap above \( T_c \). Moreover, this normal state gap function is found to be quantitatively very similar with those of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \times = 1/8 \) (\( T_c < 4K \)) in the superconducting state, pointing to a universal doping dependence of the pairing strength for \( \text{La}_x\text{CuO}_4 \)-based cuprates, which also highlights the inherent lack of a global phase coherence in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \times = 1/8 \) that makes it a failed superconductor.

1:39PM B10.00013 Quantum Oscillations in the mixed state of \( d \)-wave superconductors1, ASHOT MELIKIAN, Argonne National Laboratory. OSKAR VAFEK, National High Magnetic Field Lab and Florida State University — We show that the low-energy density of quasi-particle states in the mixed state of ultra-clean \( d \)-wave superconductors is characterized by pronounced quantum oscillations in the regime where the cyclotron frequency \( \hbar \omega_c \ll \Delta_0 \), the \( d \)-wave pairing gap. Such oscillations as a function of magnetic field \( B \) are argued to be due to the internodal scattering of the \( d \)-wave quasiparticles near wavevectors \( \pm k_D, \pm k_D' \) by the vortex lattice as well as their Zeeman coupling. The periodicity of the oscillations is set by the condition \( k_D \pm k_D' / \hbar c (eB)^{1/2} \ll \hbar c k_D / \hbar c (eB')^{1/2} \) (mod 2\( \pi \)). We find that there is additional structure within each period which grows in complexity as the Dirac node anisotropy increases.

1A. M. was supported by the U.S. Dept. of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. O.V. was supported in part by the NSF grant DMR-00-84173.

1:51PM B10.00014 Quantum Oscillations in the Underdoped Cuprate \( \text{YBa}_2\text{Cu}_3\text{O}_4 \) - EDWARD YELLAND, University of St Andrews, UK. JOHN SINGLETON, CHUCK MIELKE, NEIL HARRISON, FEDOR BALAKIREV, LANL, BOGDAN DABROWSKI, Northern Illinois University, MARCIN MATUSIAK, JOHN COOPER, University of Cambridge — The quantum oscillations (QOs) seen in the underdoped cuprate superconductor \( \text{YBa}_2\text{Cu}_3\text{O}_4 \) (\( T_c = 124K \)) in magnetic fields up to \( B = 85T \) [1] are strong evidence for a well-defined Fermi surface (FS) in \( T = 124K \) at low temperature \( T \) and high \( B \). The QO frequency \( F \approx 660 \pm 15T \), implies a FS pocket with 2.4% of the full Brillouin zone (BZ) area. Taken with earlier work [2], our data suggest FS pockets are generic to underdoped \( \text{Cu}_2\text{O}_2 \) planes and give the first hint of doping dependence of the FS. We discuss the carrier concentration implied by the QOs within various models. Comparison of the T-linear specific heat \( \gamma \) (from QO quasi-particle mass \( m^* \)) to \( \gamma \) estimated from zero-field specific heat measurements constrains the number of FS pockets present in the BZ and supports a reduced BZ due e.g. to a charge/spin density wave or ordered orbital currents. [1] E. A. Yelland et al, arXiv:0707.0057. [2] N. Doiron-Leyraud et al, Nature 446, 565 (2007)

203PM B10.00015 Fermi surface pockets in the underdoped cuprate \( \text{YBa}_2\text{Cu}_3\text{O}_4 \), are they present in low magnetic fields? , J. R. COOPER, M. MATUSIAK, J. W. LORAM, Department of Physics, University of Cambridge, E. A. YELLAND, School of Physics and Astronomy, University of St. Andrews, B. DABROWSKI, Department of Physics, Northern Illinois University — The observations of quantum oscillations in the underdoped cuprate superconductors, ortho-II \( \text{YBa}_2\text{Cu}_3\text{O}_4 \) [1] and \( \text{YBa}_2\text{Cu}_3\text{O}_4 \) (\( T_c = 124K \)) [2] at very high magnetic fields and low temperatures could lead to improved understanding of cuprate superconductivity. This will be especially true if the small Fermi surface (FS) pockets are still present at higher temperatures and lower magnetic fields. As pointed out in ref. [2] the pockets appear to have low Fermi energies \( T \approx 300 \), and could therefore give rise to T-dependent magnetic anisotropy in the normal state associated with Landau-Peierls diamagnetism. We report susceptibility measurements constrains the number of FS pockets present in the BZ and supports a reduced BZ due e.g. to a charge/spin density wave or ordered orbital currents. [1] E. A. Yelland et al, arXiv:cond-mat/07070057.

Monday, March 10, 2008 11:15AM - 1:51PM Session B11 DCMP: Magnetic Properties of Cuprate Superconductors Morial Convention Center RO9

11:15AM B11.00001 Disappearance of antiferromagnetic spin excitations in overdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) — JOHN TRANQUADA1, Brookhaven National Lab, S. WAKIMOTO, Japan Atomic Energy Agency, K. YAMADA, IMR, Tohoku Univ., C.D. FROST, ISIS Facility, RAL, R.J. BIRGENEAU, UC Berkeley, H. ZHANG, Univ. of Toronto — We have used time-of-flight neutron spectroscopy to study magnetic excitations, for energies up to \( \sim 100 \text{ meV} \), in overdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) with \( x = 0.25 \) and 0.30 [1]. Comparison of spectra integrated over the width of an antiferromagnetic Brillouin zone demonstrates that the magnetic scattering at intermediate energies, 20 < \( \omega < 100 \text{ meV} \), progressively decreases with overdoping. Previous work has shown that the low-energy magnetic excitations also disappear with overdoping [2]. This strongly suggests that the magnetism is a vestige of the parent antiferromagnet; spatial segregation of the doped holes, as in the stripe picture, provides a natural way for this to occur. Both the magnetism and superconductivity disappear as the system becomes a homogeneous metal. [1] S. Wakimoto et al., Phys. Rev. Lett. 98, 247003 (2007). [2] S. Wakimoto et al., Phys. Rev. Lett. 92, 217004 (2007).

Supported by Office of Science, US DOE, under Contract No. DE-AC02-98CH10886.

11:27AM B11.00002 Spin Susceptibility of Underdoped Cuprates: Insight from Stripe-Ordered \( \text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4 \) - MARKUS HÜCKER, GEN D. GU, JOHN M. TRANQUADA, Brookhaven National Laboratory — The low-temperature decrease of the bulk magnetic susceptibility in underdoped high-temperature superconductors has commonly been cited as evidence for a pseudogap; however, the interpretations range from a Fermi-liquid perspective, with the susceptibility being proportional to the density of free carriers, to strong coupling pictures, with the susceptibility resulting from antiferromagnetic correlations among local moments. Analysis of the susceptibility of a particular cuprate, the stripe ordered \( \text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4 \), sheds new light on this remarkable system and puts tight constraints on possible interpretations. The recently discovered magnetic transition in high magnetic fields will also be discussed.


1This work was supported by the DOE under contract number DEAC02-98CH10886.
11:39AM B11.00003 Magnetic correlations on full chains of ortho-II YBCO6.5, WEI CHEN, PETER J. HIRSCHFELD, Department of Physics, University of Florida — We propose that the $^{63}$Cu NMR line shape of chain Cu in YBCO6.5 ortho-II samples may be explained by assuming induced magnetization due to oxygen vacancies and strong correlations in the chain. The model consists of CuO chains coupled to CuO2 plane with Hubbard correlations treated in unrestricted Hartree-Fock approximation, which induce magnetic moments around oxygen chain vacancies. The broadening and shift of Pr0.5La0.5Sr2CuO4 (Pr0.5La0.5Sr2CuO4) Pr0.5La0.5Sr2CuO4 main line is consistent with increased chain magnetization at low temperature. Tunnelling between chains and the plane induces magnetization on the planar copper as well, which gives rise to quasi-1D like spin correlations in the plane.

11:51AM B11.00004 Normal state magnetic susceptibility measurements in overdoped YBa2Cu3O7−δ, BRIGITTE LERIDON, PHILIPPE MONOD, LPEM - CNRS/ESPCI - 10 rue Vauquelin -75231 Paris cedex 05 - France, DOROTHÉE COLSON, Service de Physique de l’Etat Condensé - DSM/DREAMC - CEA Saclay - 91191 Gif-Sur-Yvette Cedex - France — Motivated by the observation of staggered magnetic moments by Faquè et al. [Phys. Rev. Letters 96, 197001 (2006)] using neutron diffraction in overdoped YBa2Cu3O7−δ, we have measured the magnetization of fourteen overdoped YBa2Cu3O7−δ samples under 1 T from $T_c$ to 400 K. The oxygen contents are ranging from 6.43 to 7.00, and the critical temperatures $T_c$ from about 30 K to 91 K. We present here high resolution susceptibility data corresponding to a sensitivity of $10^{-8}$ μemu per Cu atom. We separate the different contributions to the magnetization. We find: i) a small ferromagnetic contribution, visible at all temperatures within our range of measurement and consistent with a few ppm of $F_{c2}(T)$, ii) A “1/T” paramagnetic contribution attributed to a few percent of free Cu ions, iii) The contribution of the “pseudogap” which gives a susceptibility increasing with temperature excepted in the optimally doped samples where the susceptibility is flat as expected for Pauli paramagnetism. We discuss the physical implications of this contribution in light of experiments from Faquè et al.

12:03PM B11.00005 The Persistence of High-Frequency Spin Fluctuations in Overdoped Superconducting La2−xSrxCuO4 ($x=0.22$), O.J. LIPSCOMBE, B. VIGNOLLE, S.M. HAYDEN, H.H Wills Physics Laboratory, Tyndall Avenue, Bristol, BS8 1TL, UK, D.F. MCMORROW, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London WC1E 6BT, UK, T.G. PERRING, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, UK — The wavevector and energy dependence of the spin fluctuations in overdoped superconducting La2−xSrxCuO4 ($T_c$=26 K) were investigated up to high energy (160 meV) by inelastic neutron scattering. Overdoping was found to suppress the strong magnetic response $\chi(q,ω)$ present in optimally doped La2−xSrxCuO4 which is peaked near 50 meV. The magnetic excitations were less dispersive than in the optimal compound and incommensurate at all energies investigated. Overdoping did not appear to weaken the high-frequency $E \geq 100$ meV response, suggesting that significant antiferromagnetic exchange couplings persist well into the overdoped part of the cuprate phase diagram.

12:15PM B11.00006 Conditions for magnetically induced singlet d-wave superconductivity on the square lattice1, S.R. HASSAN, B. DAVOUDI, B. KYUNG, A.-M.S. TREMBLAY, Universite de Sherbrooke — It is expected that at weak to intermediate coupling, d-wave superconductivity can be induced by antiferromagnetic fluctuations. However, one needs to clarify the role of Fermi surface topology, density of states, pseudogap, and wave vector of the magnetic fluctuations on the nature and strength of the induced d-wave state. To this end, we study the generalized phase diagram of the two-dimensional half-filled Hubbard model as a function of interaction strength $U/t$, frustration induced by second-order hopping $t''/t$, and temperature $T/t$. In experiment, $U/t$ and $t''/t$ can be controlled by pressure. We use the two-particle self-consistent approach (TPSC), valid from weak to intermediate coupling. D-wave superconductivity can be induced by magnetic fluctuations but only if they are near commensurate wave vectors and not too close to perfect nesting conditions where the pseudogap becomes detrimental to superconductivity. For given $U/t$ there is an optimal value of frustration $t''/t$ where the superconducting $T_c$ is maximum. The symmetry $d_{x^2−y^2}$ vs $d_{xy}$ of the superconducting order parameter depends on the wave vector of the underlying magnetic fluctuations in a way that can be understood qualitatively from simple arguments.

1Supported by NSERC, CRC program, CFI, MEQ, CIFAR, FQRNT.

12:27PM B11.00007 Finite size effects in NMR $T_2$ relaxation by vortex vibrations1, RACHEL WORTIS, Trent University, ERIC BROWN, SINAN BULUT — Nuclear magnetic resonance measurements are a powerful probe of electronic behavior in superconductors, but a precise understanding of all relaxation mechanisms is required to draw accurate conclusions. A previous calculation of the rate of transverse relaxation $T_2(\mathbf{r})$ present in optimally doped La2−xSrxCuO4 which is peaked near 50 meV. The magnetic excitations were less dispersive than in the optimal compound and incommensurate at all energies investigated. Overdoping did not appear to weaken the high-frequency $E \geq 100$ meV response, suggesting that significant antiferromagnetic exchange couplings persist well into the overdoped part of the cuprate phase diagram.

1Supported by NSERC of Canada, SHARCNET and Trent University.

12:39PM B11.00008 Evolution of the spin dynamics in electron-doped high-temperature superconductor Pr0.88LaCe0.12CuO4−δ ($T_c=24K$, 27K), JUN ZHAO, Department of Physics, University of Tennessee, Knoxville, TN, PENGCHENG DAI, Department of Physics, University of Tennessee, Oak Ridge National Lab, SHILIANG LI, Department of Physics, University of Tennessee, Knoxville, TN, HYE JUNG KANG, Center for Neutron Research, National Institute of Standards and Technology,Gaithersburg, MD, LOUIS-PIERRE REGNAULT, Laboratoire de Magnétisme et Diffraction Neutronique, Service de Physique Statistique, Magnétisme et Supraconductivité, PAUL STEPPENS, Institut Laue-Langevin, Grenoble, France, ARNO HIESS, instut Laue-Langevin, Grenoble, France, STEPHEN WILSON, Department of Physics, University of Tennessee, Knoxville, TN — We use both polarized and unpolarized neutron scattering to study spin excitations in electron doped cuprates Pr0.88LaCe0.12CuO4−δ($T_c=24K$, 27K). We determine the dynamic susceptibility and its temperature dependence for energies between 0.5meV to 30meV in these samples. Our results show that the spectral weight of optimal doped PLCCO (27K) around resonance energy region (~10meV) is much stronger than that of the slightly underdoped 24K PLCCO. We also demonstrate that using polarized neutrons are necessary to isolate magnetic scattering from nonmagnetic processes. A determination of the evolution of spin excitations in PLCCO as the system is tuned from nonsuperconducting to superconducting states is important to our understanding of the role of magnetism in high-Tc superconductivity.
12:51PM B11.00009 Incompatibility of Checkerboard Patterns with the Resonance Peak in Cuprate Superconductors\textsuperscript{1}. ERICA CARLSON, DAOXIN YAO, Purdue University — Checkerboard patterns have been proposed to explain STM experiments on the cuprates BSCCO and Na-COCO. However, simple checkerboard patterns are inconsistent with neutron scattering data, since they have low energy incommensurate spin peaks rotated 45° from the direction of the charge peaks.\textsuperscript{[1]} Recently, more complicated checkerboard patterns have been proposed in order to reconcile this conflict. In this work, we have studied modulated checkerboards by using spin wave theory and analyzed noncollinear checkerboards as well. We find that the high energy response of the modulated checkerboards is inconsistent with neutron scattering results, since they fail to exhibit a resonance peak at $(\pi, \pi)$ which has recently been shown to be a universal feature of cuprate superconductors. Furthermore, noncollinear checkerboards also lack a resonance peak.\textsuperscript{[2]} However, stripe patterns naturally exhibit a resonance peak consistent with neutron scattering data. References: [1] D. X. Yao, E. W. Carlson, and D. K. Campbell, Phys. Rev. B 73, 224525 (2006) [2] D. X. Yao and E. W. Carlson, arXiv:0708.1966

\textsuperscript{1}Support is acknowledged from Research Corporation.

1:03PM B11.00010 High field, low temperature 17O Knight shift in an underdoped High-Tc cuprate: La(2-x)Sr(x)CuO(4) for $x = 0.115, 0.15$. GREG BOEBINGER, ROBERT SMITH, PHILIP KUHNS, ARNEIL REYES, National High Magnetic Field Lab, TAKASHI IMAI, McMaster University — We use high magnetic fields (>30T) to suppress the superconducting Tc in order to investigate the normal state NMR properties of La(2-x)Sr(x)CuO(4) (LSCO) at low temperatures. Recent studies have shown glassy behavior and incommensurate spin-waves in LSCO, which has been discussed as evidencing a stripe ordered phase at low temperatures in the under-doped regime. We use 17O NMR as a local probe of the electron density on the planar oxygens. 17O Knight shift and linewidth were obtained over a wide temperature range in the normal state for under-doped ($x=0.115$) and optimally doped ($x=0.15$) LSCO.

1:15PM B11.00011 Static Magnetic Order in Underdoped HgBa$_2$CuO$_{4+\delta}$. YUAN LI, Stanford Univ., VICTOR BALENTED, LLB, France, NEVEN BARISTIC, Universitat Stuttgart, Germany, PHILIPPE BOURGES, LLB, France, YONGCHAN CHO, Pusan National Univ., Korea, BENOIT FAUQU, YUAN SIDIS, LLB, France, GIUCHUAN YU, Stanford Univ., XUDONG ZHAO, Jilin Univ., P. R. China, MARTIN GREVEN, Stanford Univ. — It is believed by many that understanding the pseudogap phase is essential to understanding the mechanism of high-transition-temperature superconductivity. Here we present the first experimental identification, by polarized neutron diffraction, of an exotic magnetic order in the HgO$_2$Cu$_4$ (Hg1201), which is considered the model high-Tc material with (i) simple tetragonal structure, (ii) large spacing between the CuO$_2$ planes, and (iii) the highest Tc among all single-layer compounds [1]. The parameter $\delta$ develops below a characteristic temperature $T_{\text{mag}}$ that nicely agrees with the pseudogap temperature $T^*$ determined by DC transport. Our result is highly consistent with the previous work by B. Fauque et al. on the bi-layer compound YBCO [2], and can be interpreted within an orbital-current picture that breaks time-reversal symmetry but preserves discrete translational symmetry. The magnitude and the orientation of the magnetic moments of the current loops are experimentally investigated. 1. X. Zhao et al., Adv. Mat. 18, 3243 (2006). 2. B. Fauque et al., PRL 96, 197001 (2006).

1:27PM B11.00012 Quantum Spin Excitations through the metal-to-insulator crossover in YBa$_2$Cu$_3$O$_{y+y'}$. SHILIANG LI, University of Tennessee, ZAHRA YAMANI, Chalk River Laboratories, Canada, HYE-JUNG KANG, NIST and University of Maryland, KOJI SEGAWA, YOICHI ANDO, Osaka University, Japan, XIN YAO, Shanghai Jiaotong University, China, H.A. MOOK, ORNL, PENGCHENG DAI, University of Tennessee and ORNL. — We use inelastic neutron scattering to study the temperature dependence of the spin excitations of a detwinned superconducting YBa$_2$Cu$_3$O$_{6.45}$ ($T_c = 48$K). In contrast to earlier work on YBa$_2$Cu$_3$O$_{6.5}$ ($T_c = 58$K), where the prominent features in the magnetic spectra consist of a sharp collective magnetic excitation termed “resonance” and a large ($h\omega \approx 15$ meV) superconducting spin gap, we find that the spin excitations in YBa$_2$Cu$_3$O$_{6.45}$ are gapless and have a much broader resonance. Our detailed mapping of the spin excitations along the $\gamma$-axis direction reveals a dispersion consistent with the “hourglass” like dispersion near the resonance, but the spin excitations are isotropic at lower energies. Since a fundamental change in the low-temperature normal state of YBa$_2$Cu$_3$O$_{6+y}$ when superconductivity is suppressed takes place at $y \approx 0.5$ with a metal-to-insulator crossover (MIC), where the ground state transforms from a metallic to an insulating-like phase, our results suggest a clear connection between the large change in spin excitations and the MIC.

1:39PM B11.00013 Magnetic excitations in the high-temperature superconductors HgBa$_2$CuO$_{4+\delta}$ and Nd$_{1.84}$Ce$_{0.155}$CuO$_4$. GIUCHUAN YU, YUAN LI, EUGENE MOTOYAMA, Stanford University, PHILIPPE BOURGES, Laboratoire Léon Brillouin, KLAUDIA HRADIL, RICHARD MOLE, Forschungszentrum Jülich, Heinz Maier-Leibnitz, MARTIN GREVEN, Stanford University — We report inelastic neutron scattering results for the magnetic excitations in hole-doped HgBa$_2$CuO$_{4+\delta}$ (Hg1201) and electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4+\delta}$ (NCCO). The magnetic resonance mode has been observed previously in the superconducting state of several hole-doped systems. Recently, this mode has also been claimed to be present in the electron-doped compounds. We found in underdoped Hg1201 ($T_c \approx 95$K) the resonance-like feature appearing at rather high energy of 57(2)meV. Surprisingly, the dynamic susceptibility enhancement appears below the pseudogap temperature $T^*$ and shows no anomaly at $T_c$. Unlike recent reports for optimally-doped NCCO and (PrLaCe)$_2$CuO$_{4+\delta}$, we found no evidence for a resonance mode in NCCO ($x=0.155$) in the 7-12 meV range. Instead, we identify two lower-energy features. One is associated with spectral weight redistribution below $T_c$ due to the electronic gap $2\Delta$, the other already present in normal state is likely associated with the significant spin correlations in the electron-doped cuprates.

Monday, March 10, 2008 11:15AM - 2:03PM –
Session B12 DCMP: Organic Conductors and Strongly Correlated 2D Systems Morial Convention Center 203

11:15AM B12.00001 The metal insulator transition in correlated quasi-one-dimensional organic conductors\textsuperscript{1}. CLAUDE BOURBONNAIS, ABDELOUAHAB SEDEKI, Departement de Physique, Universite de Sherbrooke, Sherbrooke (QC), Canada J1K-2R1 — We use a two-loop functional renormalization group approach to calculate the quasi- particle weight along the Fermi surface in the framework of the quasi-one- dimensional electron gas model which includes weak Umklapp scattering at half-filling. The location and evolution of cold and hot spots for electron-electron scattering is described and the Fermi surface reconstruction is clarified as a function of the amplitude of Umklapp scattering. The results are applied to the Mott transition in the Fabre salts series (TMTTF)$_2$X where the emergence of a Fermi surface is found as a consequence of electronic deconfinement under the application of hydrostatic pressure.

\textsuperscript{1}Supported by NSERC and the Canadian Institute of Advanced Research.
11:27AM B12.00002 Numerical Study of Finite-Temperature Phase Transitions in Quasi-One-Dimensional Molecular Conductors, YUCHI OTSUKA, CREST-JST, JAE/A/SPRING-8, HITOSHI SEO, JAE/A/SPRING-8, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo, TAKEO KATO, Institute for Solid State Physics, University of Tokyo — We have theoretically investigated the charge ordering, the dimer Mott, and the spin-Peierls phase transitions in quarter-filled quasi-one-dimensional organic conductors, such as DCNQI$_2$X and TMTTF$_2$X, by considering the extended Hubbard model with electron-lattice couplings and inter-chain Coulomb interaction. We apply the stochastic-series-expansion quantum Monte Carlo method to the effective one-dimensional model obtained by the adiabatic and inter-chain mean-field approximation. We discuss the competition of the order parameters and the susceptibilities are calculated for the charge ordering, the dimer Mott, and the spin-Peierls transitions. The results show a competition between the charge-ordered and dimer Mott insulating states, consistent with our previous work [1], and both of them undergo the spin-Peierls transition at low temperatures. There, two types of spin-Peierls phases with spin gap appear in competition with showing different orderings of period four in lattice distortion and charge disproportionation. [1] H. Seo, Y. Motome, and T. Kato, J. Phys. Soc. Jpn. 76, 013707 (2007).

11:39AM B12.00003 High field ESR on tau phase conductor —from GHz to THz—, TAKAHIRO TOKUMOTO, J. VAN TOL, L.-C. BRUNEL, D. GRAF, J.S. BROOKS, FSU/NHMFL, Y. OSHIMA, IMR, Tohoku Univ., G. PAPAVASSILIOU, NSW, Greece — Organic conductors have exotic electronic and magnetic properties ranging from the possibility of unconventional, anisotropic superconductivity, to the observation of a variety of ground states such as charge-density waves, spin-density waves, field-induced spin density waves, and the observation of quantum Hall effect, or a spin-Peierls state. One example is tau - [P-(S,S) - DMEDT-TTF)(AuBr2)]$_1$ y (-0.75). The crystal structure of this quasi two dimensional organic compound is tetragonal with unit cell dimensions: a = 7.3546 A and c = 67.977 A. Even though there are no magnetic ions in the system, several measurements indicate magnetic ordering at low temperature and under magnetic fields. Furthermore, this compound exhibits field induced hysteretic MI transition above 38T with an inking of weak ferromagnetism. We investigate the origin of the magnetic behavior by conducting a CW ESR study from 90GHz to 1.2 THz. Results and analysis will be presented.

12:03PM B12.00005 Charge frustration and novel electron-lattice coupled phase transition in organic conductor DI-DCNQI$_2$Ag, HITOSHI SEO, JAE/A/SPRING-8, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — We have theoretically investigated the phase transition accompanying charge ordering in 1/4-filled quasi-one-dimensional organic conductor DI-DCNQI$_2$Ag. The nature of this phase transition at 220 K has been under debate since the first direct observation of charge ordering among organic quasi-one-dimensional systems by Hiraki and Kanoda[1]. In this study, motivated by a recent synchrotron radiation x-ray study by Kakiuchi et al.[2], we investigate a three-dimensional interacting spinless fermion model coupled to the lattice degree of freedom. We have found that the peculiar “spiral frustration” existing in the interchain Coulomb interaction destabilizes simple Wigner crystal-type charge order and gives rise to a novel state where different chains show different orders and align periodically: charge order, lattice dimerization, and a co-existence of them. The co-existence of these two orders was in fact predicted in our previous study for the non-frustrated case[3], which was stabilized as a result of competing interactions. In contrast, the co-existence in the present study is obtained by compromising the frustration in charge sector. [1] K. Hiraki and K. Kanoda, Phys. Rev. Lett. 80 (1998) 4737. [2] T. Kakiuchi et al., Phys. Rev. Lett. 98 (2007) 066402. [3] H. Seo, Y. Motome, and T. Kato, J. Phys. Soc. Jpn. 76 (2007) 013707.

12:15PM B12.00006 Finite size effects in micro- and nanocrystals of (TMTSF)$_2$ClO$_4$, P. DHAKAL, J.I. OH, M.J. NAUGHTON, Boston College — We report transport measurements in micro- and nano-sized crystals of the molecular organic (super)conductor (TMTSF)$_2$ClO$_4$. Synthesized using the standard electrocrystallization process, various techniques such as focus ion beam-induced metallization, photo lithography, and atomic layer deposition were then employed to successfully make micro- and nano-electrodes contacting these samples. In addition, FIB sculpting was used to reshape crystals to reduce their sizes. We have successfully measured crystals with dimensions as small as 300 nm. We have observed that electrical transport behaviors of these finite sized crystals are very different from those of their parent bulk crystals. We will discuss our observations in terms of various origins such as finite size effects, fabrication-induced defects, and combinations thereof.

12:27PM B12.00007 Pulsed-field study of the interference commensurate effect in quasi-one-dimensional organic conductors, J. ROY, J.I. OH, H. YOSHINO, P. DHAKAL, M.J. NAUGHTON, Boston College — We report angle-dependent magnetoresistance oscillations for fields up to 43 T oriented mainly in the most conducting x-y plane, with small field component along the least conducting z axis, in the q1d compounds (TMTSF)$_2$ClO$_4$ and (DMET)$_2$I$_3$ at 1.5 K. A hybrid plastic-metal cryoprobe system with pseudo dual-axis rotation has been built for these pulsed-field measurements. Due to the interference commensurate effect, (aka Lee-Naughton oscillations) [1-3], we have observed rich magnetoresistance oscillations, resulting from an interference effect of commensurate electron trajectories in the extended Brillouin zone. Also, we have found that, as theoretically expected [2], field-dependent magnetoresistence shows 1D and 2D transport behavior at local resistance maxima and minima (versus field angle), respectively. Temperature dependences of the order parameters and the susceptibilities are calculated for the charge ordering, the dimer Mott, and the spin-Peierls transitions. The results show a competition between the charge-ordered and dimer Mott insulating states, consistent with our previous work [1], and both of them undergo the spin-Peierls transition at low temperatures. There, two types of spin-Peierls phases with spin gap appear in competition with showing different orderings of period four in lattice distortion and charge disproportionation. [1] J.J. Lee and M.J. Naughton, Phys. Rev. B 57, 7423 (1998). [2] A.G. Lebed, et al., Phys. Rev. Lett. 91, 187003 (2003). [3] H.I. Ha, et al., Phys. Rev. B 73, 033107 (2006).

1This work was supported by NSF Grant No. DMR 0605339.
2Permanent address: Osaka City University.
12:39PM B12.00008 Acoustic properties of quasi-one-dimensional organic conductor (TMTSF)$_2$ClO$_4$ in the relaxed state: Superconductivity and FISDW anomalies. ALEXANDRE LANGLOIS, MARIO POIRIER, CLAUDE BOURBONNAIS, Universite de Sherbrooke, KLAUS BECHGAARD, Risoe National Laboratory — Through competing electronic instabilities, the anion sublattice plays an important role in the nematic phase diagram of the Bechgaard salts. In the quasi-one-dimensional organic conductor (TMTSF)$_2$ClO$_4$, anion ordering at 24 K affects the nesting properties of the Fermi surface and controls the stability of the superconducting phase below 1.2 K at ambient pressure. Moreover, the field induced spin density wave phases FISDW, one of the several features induced by a magnetic field in this compound, are also sensitive to the symmetry of the anions. In order to address the coupling issue between the lattice and these electronic instabilities, we have performed the first ultrasonic measurements on (TMTSF)$_2$ClO$_4$ in the relaxed state below 4 K using longitudinal and transverses waves (30-500 MHz). If low-frequency vibrating reed experiments have revealed magneto-elastic anomalies in the FISDW phases [1], the superconducting one was never investigated by similar techniques. We report anomalies in the ultrasonic velocity and attenuation for the superconducting and the FISDW phases. The coupling of these phases to the lattice is discussed in relation with the known T-B phase diagram. [1] X.D. Shi et al., Phys. Rev. B. 50, 1984 (1994).

12:51PM B12.00009 Spin dynamics of the field-induced spin density wave phases in (TMTSF)$_2$ClO$_4$ in tilted magnetic fields. L.L. LUMATA, J.S. BROOKS, A.P. REYES, P.L. KUHNS, Department of Physics and National High Magnetic Field Laboratory, Florida State University, S.E. BROWN, Department of Physics, UCLA, H.B. CUI, Department of Physics and National High Magnetic Field Laboratory, Florida State University, J.-I. TAMADA, Department of Material Science, University of Hyogo — The spin dynamics of the different subphases of the field-induced spin density wave (FISDW) ground state in (TMTSF)$_2$ClO$_4$ was investigated using simultaneous $^{77}$Se nuclear magnetic resonance (NMR) and electrical transport. The metallic and FISDW phases were accessed by rotating the sample along its most conducting axis in a constant magnetic field $H$ and constant temperature. At a fixed field of 30 T and constant temperature 1.47K, we report observation of divergence in the spin-lattice relaxation rate $1/T_1$ at angles corresponding to $H_z = H \cos(\theta) \sim 6.4T, 15.9T,$ and 26T phase transitions. There is a gradual increase in $1/T_1$ in the 2nd-order/FISDW cascade region and a nearly metallic-like behavior deep in the final reentrant SDW phase is observed. rf enhancements in the metallic and FISDW phases were also measured. The details will be discussed.

1Work supported in part by NSF-DMR 060289; NHMFL supported by the NSF and the State of Florida.

1:03PM B12.00010 Interlayer Cooperon correction to angular-dependent magnetoresistance in layered metals. MALCOLM KENNEDIT, Simon Fraser University, ROSS MCKENZIE, University of Queensld — Studies of angle-dependent magneto-resistance oscillations (AMRO) in the interlayer conductivity of layered metals have generally considered semi-classical electron transport. We consider a quantum correction to the semi-classical conductivity which arises from what can be described as an interlayer Cooperon. This depends on both the disorder potential within a layer and the correlations of the disorder potential between layers. We compare our results with existing experimental data on organic charge transfer salts that is not explained within the standard semi-classical transport picture. In particular, our results may be relevant for weak localization-like effects that have been seen when the applied magnetic field is close to parallel to the conducting layers.

1:15PM B12.00011 Coulomb drag at zero temperature. ALEX LEVCHENKO, ALEX KAMENEV, University of Minnesota — We show that the Coulomb drag effect exhibits saturation at small temperatures, when calculated to the third order in the interlayer interactions. The zero-temperature transresistance is inversely proportional to the third power of the dimensionless sheet conductance. The effect is therefore the strongest in low mobility samples. This behavior should be contrasted with the conventional (second order) prediction that the transresistance scales as a certain power of temperature and is almost mobility-independent. The result demonstrates that the zero-temperature drag is not an unambiguous signature of a strongly-coupled state in double-layer systems.

1:27PM B12.00012 Collective modes in quantum electron glasses and electron-assisted hopping. MARKUS MUELLER, Harvard University, LEV IOFFE, Rutgers University — We study electronic transport in Anderson insulators with strong Coulomb interactions in dimensions $d \geq 2$. Close to the metal insulator transition where the single particle localization length is much larger than interparticle-distance, the interactions lead to a strongly correlated quantum glass phase. Even though single particle excitations are localized and the system is insulating, there are collective electronic modes which remain delocalized down to parametrically small energies. These collective excitations serve as a continuous bath which can provide the activation energy for variable range hopping transport. This circumvents the energy conservation problem arising when only discrete particle-hole excitations are present. In contrast to the weak and material-dependent phonon-assisted hopping mechanism, the activation by an electronic bath leads to a nearly universal prefactor $e^2/h$ of the Efros-Shklovskii conductance, as is observed in many recent experiments.

2This work was supported by Swiss National Science Foundation grant PA002-113151, ARO grant W911NF-06-1-0208 and NSF grant ECS 0608842.

1:39PM B12.00013 Hall effect on the triangular lattice. GLADYS LEON, CHRISTOPHE BERTHOD, THIERRY GIAMARCHI, DPMC-MaNEP, University of Geneva, 24 quai Ernest-Abnsermet, 1211 Geneva 4, Switzerland., ANDREW MILLIS, Department of Physics, Columbia University, 538 West, 120th Street, New York, NY 10027, USA — We investigate the Hall effect on the two-dimensional triangular lattice. We calculate the high frequency Hall constant $R_H$ and its temperature dependence for three regimes of the Hubbard interaction $U$. In the non-interacting case $U=0$ we find that $R_H$ behaves at temperature $T=0$ like the classical dc Hall constant, $R_H \sim 1/\pi e$. At high $T$ we find a positive $R_H$ increasing linearly with temperature, with a slope depending on the electron density. For small to moderate values of $U$, we study the effect of interactions on $R_H$ within second-order perturbation theory, and we find these effects to be small. The perturbation theory also shows that the electron self-energy is almost local ($k$-independent), suggesting the use of a local approximation as the Dynamical Mean Field Theory (DMFT) method to treat higher values of $U$. We therefore evaluate $R_H$ at large $U$ using both DMFT and the atomic limit of the self-energy, and we compare the results with those obtained at small $U$. Finally, we discuss the relevance of our calculations for the interpretation of recent Hall measurements in cobaltates.

2This work was supported by the Swiss National Science Foundation through Division II and MaNEP.

1:51PM B12.00014 Quantum Phase Transition in a Cold Atomic Spin-Boson Mixture. PETER P. ORTH, IVAN STANIC, KARYN LE HUR, Yale University — We theoretically implement a spin array in a tunable bosonic environment using cold bosonic atoms with two (hyperfine) ground states, trapped by different potentials [1]. The first specie lies in a deep optical lattice with tightly confining wells and the second specie forms a superfluid reservoir. Different species are coupled coherently via laser transitions and collisions. Whereas the laser coupling mimics a transverse field for the spins, the coupling to the reservoir phonons (sound modes) induces a ferromagnetic (Ising) coupling as well as dissipation. This results in a peculiar ferro-paramagnetic quantum phase transition where the effect of dissipation can be studied in a controllable manner.

Monday, March 10, 2008 11:15AM - 2:03PM –
Session B13 DCOMP GSCCM: Focus Session: Simulations of Matter at Extreme Conditions
II: Beryllium, Carbon, and Metals
Morial Convention Center 204

11:15AM B13.00001 The Role of Anharmonicity in the Beryllium Equation of State, LORIN X. BENEDICT, ANDREA TRAVE, CHRISTINE WU, TADASHI OGITSU, PHIL STERNE, ERIC SCHWEGLER, Lawrence Livermore National Lab, H-DIV COLLABORATION — We discuss the construction of a multi-phase equation of state for Be from first principles, aimed at understanding the material’s properties at extreme conditions. In addition to the usual computation of cold, quasiharmonic ion-thermal, and (negligible here) electron-thermal contributions, we consider the effects of strong anharmonicity in the bcc phase, and argue that the inclusion of such effects may greatly perturb the picture (in particular, the phase diagram) derived from assuming quasi-harmonic lattice dynamics. Our analysis involves studying the mean displacement from equilibrium of Be atoms in the lattice by DFT-molecular dynamics methods and comparing the results to those of the quasiharmonic theory.

11:27AM B13.00002 Quantum molecular dynamics simulations of beryllium at high pressures1, MICHAEL DESJARLAIS, MARCUS KNUDSON, Sandia National Laboratories — The phase boundaries and high pressure melt properties of beryllium have been the subject of several recent experimental and theoretical studies. The interest is motivated in part by the use of beryllium as an ablative material in inertial confinement fusion capsule designs. In this work, the high pressure melt curve, Hugoniot crossings, sound speeds, and phase boundaries of beryllium are explored with DFT based quantum molecular dynamics calculations. The entropy differences between the various phases of beryllium are extracted in the vicinity of the melt curve and agree favorably with earlier theoretical work on normal melting. High velocity flyer plate experiments with beryllium targets on Sandia’s Z machine have generated high quality data for the Hugoniot, bulk sound speeds, and longitudinal sound speeds. This data provides a tight constraint on the pressure for the onset of shock melting of beryllium and intriguing information on the solid phase prior to melt. The results of the QMD calculations and the experimental results will be compared, and implications for the HCP and BCC phase boundaries of beryllium will be presented.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US DOE’s NNSA under Contract No. DE-AC04-94AL85000.

11:39AM B13.00003 Equation of state of beryllium from first-principles calculations, ANDREA TRAVE, LORIN BENEDICT, TADASHI OGITSU, CHRISTINE J. WU, PHILIP A. STERNE, ERIC SCHWEGLER, Lawrence Livermore National Lab — The design of experiments of materials at extreme conditions of pressure and temperature is often based on hydrodynamic simulations, which make use of equation of state (EOS) models for the description of the systems under study. The validity of these models is extremely critical, and first-principles calculations can provide consistent and accurate parameters for the determination of the EOS in a wide range of thermodynamic conditions. Extensive density functional theory calculations at zero temperature have been performed for beryllium in various solid structures, in order to obtain accurate predictions for their compression curves, and phonon and electronic densities of states. Finite-temperature simulations have been used to further improve the models to include anharmonic effects. The melting line of beryllium has been obtained with first-principles two-phase simulations, which enables the construction of a multi-phase EOS for both liquid and solid beryllium. The results of these simulations provide useful indications on the relative stability of the various solid and liquid phases of beryllium in a region of the phase diagram lacking any experimental study so far. Prepared by LLNL in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

11:51AM B13.00004 Construction of a multi-phase equation of state for carbon at extreme pressures1, ALFREDO A. CORREA, University of California at Berkeley and Lawrence Livermore National Laboratory, LORIN X. BENEDICT, Lawrence Livermore National Laboratory, STANIMIR A. BONEV, Dalhousie University, Halifax, Canada, DAVID A. YOUNG, Lawrence Livermore National Laboratory, ERIC SCHWEGLER, Livermore National Laboratory — We describe the construction of a multi-phase equation of state for carbon at extreme pressures that is based on the results of first principles electronic structure calculations. Two solid phases (diamond, B6) and the liquid are considered. Solid-phase free energies are built from a knowledge of cold curve and phonon calculations, together with first principles molecular dynamics calculations of the equation of state itself to extract anharmonic terms. The liquid free energy is constructed from a combination of molecular dynamics calculations and constraints determined from previously calculated melt curves, assuming a simple solid-like free energy model. The resulting equation of state is extended to more extreme densities and temperatures with a plasma-based free energy model. Comparisons to available experimental results are discussed.

1Prepared by LLNL under Contract DE-AC52-07NA27344.

12:03PM B13.00005 Clustering in dense molten lithium, ISAAC TAMBLYN, Dalhousie University, JEAN-YVES RATY, University of Liege, STANIMIR A. BONEV, Dalhousie University — Molten lithium is investigated from zero to over nine-fold compression using first principles theory. Over this pressure range, we observe several electronic and structural transitions. The changes that lithium undergoes with increasing pressure are initially analogous to those predicted for liquid sodium [1]. However, upon further compression, effects due to increased core overlap lead to a new liquid phase composed of weakly bound lithium clusters. The properties of the proposed new liquid phases, the melting curve of lithium, and the implications of our findings for the stability of low-symmetry lithium solids will be discussed. [1] J.-Y. Raty, E.R. Schwegler, S.A. Bonev, Nature, 449, 448-451 (2007)

1Work supported by the NSERC of Canada

12:15PM B13.00006 Lithium at ultra-high pressures, ANDRE KIETZMANN, RONALD REDMER, Univeritat Rostock, Institut fur Physik, D-18051 Rostock, Germany, MICHAEL P. DESJARLAIS, THOMAS R. MATTSION, Sandia National Laboratories, Albuquerque, NM 87185-1186, USA — Lithium is a prototypical simple metal at standard conditions. However, by changing the density towards expanded or compressed states, the electrical conductivity shows strong variations. We have performed quantum molecular dynamics simulations for fluid lithium covering a wide range of densities and temperatures in order to derive the equation of state, the electrical conductivity, and information about structural and electronic changes along the expansion or compression. The electrical conductivity changes from the nonmetallic expanded fluid via the fluid metal region up to the degenerate electron liquid at high densities. We find a largely ordered ion structure at ultra-high densities reflecting a multi-centered ion situation in the liquid as predicted earlier for solid lithium. Supported by the DFG within SFB 652. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:27PM B13.00007 ABSTRACT WITHDRAWN –
12:39PM B13.00008 Optical Properties of LiH From Mixing Rules. DANIEL HORNER, JOEL KRESS, LEE COLLINS, Theoretical Division, Los Alamos National Laboratory — We investigate the use of pressure and density matching mixing rules for predicting the optical properties and equation-of-state (EOS) of lithium hydride for densities from half to twice solid [0.78 g/cc] and temperatures from 0.5 to 3.0 eV. The mixing rules allow us to perform simulations of lithium and hydrogen separately and, from them, calculate properties of the mixture. Using the VASP code, we performed constant (N, V, T) quantum molecular dynamics simulations for H, Li, and LiH with the results for the mixture (LiH) as a benchmark of the mixing procedures. A finite-temperature density functional theory formulation produces the electronic wave function at each time step within the generalized gradient approximation with projector augmented wave pseudopotentials. Optical properties were determined using the electronic wave function in a Kubo-Greenwood formula. We compare the frequency-dependent absorption coefficient, Rosseland Mean Opacity, and EOS computed via the mixing rules and those from a full LiH simulation.

12:51PM B13.00009 First principles investigation of the dielectric function of gold under ultrafast laser excitation¹, TADASHI OGITSU, LLNL, DAVID PRENDERGAST, LBL, ERIC SCHWEGLER, YUAN PING, ANDREW NG, LLNL — Recently, a quasi-steady state in ultrathin, ~30 nm gold foils exposed to an ultrafast laser pulse has been observed, which includes an enhanced interband transition peak at 2.6 eV in the imaginary part of the dielectric function [1]. Simulations of this system assuming a two-temperature model for the electronic and ionic degrees of freedom do not provide this enhancement in optical absorption, possibly indicating that both of these degrees of freedom are not in equilibrium. Our approach is to treat this as an inverse problem: to reproduce experiment by sampling various states of electrons and ions. We employ an efficient first principles technique to quickly estimate the dielectric function of this fcc metal for various finite temperature and non-equilibrium model distributions. Converged Brillouin zone sampling is achieved using a compact k-dependent Hamiltonian derived from first principles calculations [2]. [1] Y. Ping et al., Phys Rev Lett 96, 25503 (2006). [2] E. L. Shirley, Phys Rev B 54, 16464 (1996).

³Work at the Molecular Foundry was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Prepared by LLNL under Contract DE-AC52-07NA27344.

1:03PM B13.00010 High pressure lattice dynamics and elasticity of transition metals. DANIEL ORLIKOWSKI, LORIN BENEDICT, JOHN KLEPEIS, Lawrence Livermore National Laboratory — For continuum-level description of transition metals using equation of state and strength models, a high-pressure lattice dynamics effort is required. We present here a subset of that work to provide Debye temperatures and elastic moduli for the equation of state (EOS) and strength models. DFT calculations for the phonons are performed to obtain the Debye temperature over the pressure range required by the EOS model. For the strength model, we have combined several sets of quantum-based, atomistic calculations with density functional theory (DFT) to develop elastic moduli over a wide range of temperatures (12,000 K) and pressures (4 Mbar). Our focus is upon vanadium but other transition metals will be presented tantalum and molybdenum. Our results are comparable to available experimental data. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

1:15PM B13.00011 A new wide-range equation of state for tungsten. JOHN H. CARPENTER, Sandia National Laboratories, MICHAEL P. DESJARLAIS, ANN E. MATTSSON, KYLE R. COCHRANE — A new wide-range equation of state for tungsten is described. Quantum molecular dynamics calculations in the warm dense matter region are combined with other experimental and theoretical calculations, providing a set of information on which to tune a model of the free energy landscape. The resulting model, describing the liquid, gas, and bcc solid phases, provides a good description of the liquid-vapor critical point, melt curve, static compression data, isobaric expansion data, and the Hugoniot. Finally, improvements in table generation greatly improve the resolution of phase boundaries.

1:27PM B13.00012 ABSTRACT WITHDRAWN —

1:39PM B13.00013 Pressure Induced Solidification of Ta and Cu: A Comparison. DAVID RICHARDS, JAMES GLOSILI, FREDERICK STREITZ, Lawrence Livermore Natl Lab — Using powerful computers such as Blue Gene/L it is now possible to use classical molecular dynamics to simulate pressure induced solidification at size scales that are free of finite size effects. We present a comparison of the nucleation, growth, and coalescence of clusters during pressure induced solidification in large scale MD simulations of liquid Ta and Cu. We extract growth and nucleation rates from our simulations, as well as cluster size distributions that can be compared against the predictions of simple models. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

1:51PM B13.00014 New Phase Diagram of Ta: Bridging Laser Heated Diamond-Anvil Cell and Shock Melting³, CHRISTINE J. WU, PER A. SÖDERLIND, JAMES N. GLOSILI, JOHN E. KLEPEIS, Lawrence Livermore National Laboratory — Determination of the melt line of materials under high pressures is essential for establishing its phase diagrams and has important implications for geophysics, material science, and high-pressure physics. So far, melting temperatures at high pressure are primarily measured by in situ laser-heated diamond-anvil cell (DAC) or shock wave experiments. Often, these two methods yield significantly different results, particularly for non close-packed metals, such as bcc metals. For instance, anomalously flat melting slopes were reported for numerous bcc metals by laser-heated DAC. The flatness of the melting slope is in sharp contrast to the classical Lindemann behavior which shock-melting temperatures follow closely. In this presentation, we will report a novel phase diagram of Ta obtained from ab initio methods, and molecular dynamics (MD) simulations, which resolves the long-standing controversy, and has significant impact on our understanding of phase diagrams of bcc metals.

³This work preformed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Monday, March 10, 2008 11:15AM - 2:03PM —
Session B14 DAMOP: Casimir Forces, Collisions and Atomic Structure  Morial Convention Center 205
Numerically calculate the Casimir force on a piston in a periodically driven micromachined torsional oscillator, yielding a highly sensitive measurement of the force gradient for separations between 80nm and 500nm.

In our experiment, the force gradient is measured by the frequency shifts caused by Casimir force in the response of the crystal surfaces versus the case in which they are parallel to the surfaces. We compute the force numerically for cases of experimental interest, and discuss the orientation of the optical axes. For strongly anisotropic crystals, the Casimir force can be substantially different when the optical axes are perpendicular to the crystal surfaces versus the case in which they are parallel to the surfaces. We compute the force numerically for cases of experimental interest, and discuss the prospects for observing this effect.

We present measurements of the Casimir force gradient between a gold-coated sphere and a highly doped silicon plate with an array of nanoscale, high-aspect-ratio trenches. The Casimir force arises from quantum fluctuation of electromagnetic fields in vacuum and is strongly dependent on the boundary condition. While the majority of the precise measurements have been performed on simple arrangements of plate-shaped objects, few experiments have been done in geometries with interactions that deviate significantly from the pair-wise summation of two-body potentials. We choose one of the interacting surfaces to be an array of trenches with widths ranging from 200 nm to 500 nm and depth of 1μm. Theoretical analysis predict that for perfectly conducting surfaces with such geometry, the Casimir force differs by up to 70% from the pair-wise summation of two-body potentials. We show that large corrections to these approximations could be measured using present-day technology with a BEC used as a vacuum field sensor. For details, see D.A.R. Dalvit et al, arXiv:0710.5249, 0709:2095.

We present measurements of the Casimir force gradient between a metal and a dielectric in fluid. The boundary conditions on these fields are dependent upon the electromagnetic properties of the interacting materials and affect both the magnitude and sign of the resulting force. We will discuss our experiments for measuring the Casimir-Lifshitz force between a metal and a dielectric immersed within a fluid and will describe situations which can give rise to a repulsive interaction.

On the repulsive Casimir force using metamaterials. We discuss as realistically as possible the role that metamaterials play in the Casimir force and bring to the surface some aspects of this issue that were previously rarely mentioned, such as the typical anisotropy of metamaterials and the presence of a Drude background in its electric permittivity. We also study the Casimir and Polder force between an atom and a metamaterial, since this setup may be more suitable to the detection of repulsion forces.
Spin depolarisation of $\text{N}_2^+$ ($^2\Sigma^+$) in collisions with $^3\text{He}$ and $^4\text{He}$ in a magnetic field. TIERRY STOECKLIN, GRÉGOIRE GUILLOIN, ANATOLI VORONIN — The possibility of tuning the interactions between atoms and molecules using a magnetic field has open new possibilities of controlling collisional energy transfer at very low temperature. In a first study dedicated to $\text{He}-\text{N}_2$ inelastic collisions we found that spin free collisions of $\text{N}_2^+$ with $^3\text{He}$ and $^4\text{He}$ exhibit a strong isotope effect in the ultra cold regime, and recently found a similar effect for another ionic system: the He-CH$^+$ collision. In the present work, we compare first in the absence of an applied magnetic field the cross sections for the transitions changing the projection of the total angular momentum of $\text{N}_2^+$ ($^2\Sigma$) in collisions with $^3\text{He}$ and $^4\text{He}$ at very low collision energy. In the second part of this contribution we investigate the effect of an applied magnetic field and compare the results obtained for the fundamental states of the two nuclear spin isomers of $\text{N}_2^+$. As a result of the different mechanisms of action of the spin rotation interaction for these two rotational levels we find a great difference of sensitivity to the applied magnetic field. Whereas even moderate values of the applied magnetic field (10 Gauss) completely modify the very low collision energy behaviour of the spin depolarisation cross section of the fundamental ortho level, we find that one has to apply magnetic fields two orders of magnitude larger to obtain similar effects for the fundamental para level.


III-3PM B14.00010 Observation of the (n$^3\text{He},t)p$ Reaction by Detection of Far-Ultraviolet Radiation. CHARLES W. CLARK, Joint Quantum Institute, NIST and the University of Maryland, ALAN K. THOMPSON, National Institute of Standards and Technology, MICHAEL A. COPLAN, JOHN W. COOPER, Institute for Physical Science and Technology, University of Maryland, PATRICK HUGHES, Department of Physics, University of Maryland, ROBERT E. VEST, Electron and Optical Physics Division, National Institute of Standards and Technology — We have detected Lyman alpha radiation as a product of the n($^3\text{He},t)p$ nuclear reaction, induced in a $^3\text{He}$ gas cell irradiated by a cold neutron beam at the NIST Center for Neutron Research. The predominant source of this radiation appears to be decay of the 2p state of tritium produced by charge transfer and excitation collisions with the background $^3\text{He}$ gas. For atmospheric pressure and room temperature in the $^3\text{He}$ cell, we find yields of tens of Lyman alpha photons for every neutron reaction. These results suggest a method of cold neutron detection that is complementary to existing technologies that use proportional counters. In particular, this approach may provide single neutron sensitivity with wide dynamic range capability, and a class of neutron detectors that are compact and operate at relatively low voltages.

Photo-Fragmentation of Lithium Atoms in FEL Radiation Fields, MATTHEW FOSTER, J. COLGAN, Los Alamos National Laboratory, Theoretical Division, M.S. PINDZOLA, Auburn University, ALEXANDER DORN, Max-Planck-Institut für Kernphysik — Multi-electron ejection from lithium induced by absorption of a single photon is a fundamental few-body reaction that tests the correlated interaction dynamics between atomic constituents. Experiments have been proposed using intense FEL radiation at FLASH in combination with reaction microscopes to measure four-body dynamics. These proposed experiments will first measure the double ionization dynamics from both the even parity Li ground state and the laser excited odd parity Li(2p$^2P^o$) state. We will present theoretical calculations using the time-dependent close-coupling method (TDCC) to assist in the experimental search for interesting correlation effects for both double and triple ionization of lithium.

Long range anions: diatomic, triatomic and polyatomic molecules. EDWARD C. CHEN, The Wentworth Foundation, EDWARD S. CHEN, Baylor College of Medicine — The observation of both long range and valence anions of O$_2$, NO, CS$_2$, NO$_2$, O$_3$, SF$_6$, C$_2$F$_6$, CH$_3$NO$_2$, tetracene, anthracene, acridine, perylene, pyrene, naphthalene and the nucleobases is reported in negative ion mass spectrometry, photoionization, electron impact in nanodroplets, electron swarm experiments at low temperature and alkali metal beam studies. New polarization or quadrupole bound electron affinities less than 0.1 eV are reported for the aromatic hydrocarbons, O$_2$, SF$_6$, CS$_2$, C$_2$F$_6$ while dipole bound values less than 0.15 eV are reported for the nucleobases, NO$_2$ and NO. The long range states act as gateways to valence states. This relationship is illustrated by Morse potential energy curves in single bond dissociations and in reaction coordinates analogous to Marcus parabolas. New adiabatic electron affinities values less than 0.15 eV are reported for the nucleobases, N$_2$, O$_2$, and NO. The long range states act as gateways to valence states. This relationship is illustrated by Morse potential energy curves in single bond dissociations and in reaction coordinates analogous to Marcus parabolas. New adiabatic electron affinities are reported for some of these molecules, including (in eV) guanine, 1.64(2) adenine, 1.09(2); C$_2$F$_6$, 1.26(5); acridine, 1.09(2); perylene, 1.09(2); tetracene, 1.10(2); naphthalene, 0.19(2) eV.

The Wentworth Foundation.

The Effect of Birth Location in an Intense Laser Focus on the Non-Sequential Double Ionization Yield. JAY PAQUETTE, JAN CHALoupKA, College of William and Mary — Atoms in an intense laser field can become doubly ionized through a direct process known as rescattering, where a single electron is liberated through tunnel ionization and is driven back to the ion core by the laser field, leading to impact ionization and release of a second electron. In this quasi-classical description, the trajectory of the first electron will have a strong influence on the probability of release of a second electron, as evidenced by the reduction in yield with elliptical laser polarization. Even with linear polarization, the first electron can avoid a reencounter with the ion due to the v x B term or the longitudinal electric field component (E$_z$) in the laser focus. Since the E$_z$ term is given from the requirement of zero divergence of the electric field, its magnitude will vary as a function of position within the laser focus. Using completely classical 3-D simulations, we demonstrate how longitudinal electric field variations affect electron trajectories, how the ion yields from various regions within the focus are affected, and the likelihood of observing this effect experimentally.
Austrian Academy of Sciences, ANTON ZEILINGER, IQOQI; Faculty of Physics, University of Vienna — We successfully transmitted both photons of various link key distribution involving phase reference beams. Based on coherent states and homodyne detection is used to illustrate the method. A possible test for the quantum nature of memories using two non-orthogonal values in conjunction with the partial transposition map. Our method is designed to reduce the resources for entanglement verification. A particular protocol quantum behavior can be phrased as the verification of effective entanglement. Necessary separability criteria are formulated in terms of a matrix of expectation of quantum information processing devices, such as quantum memories, teleportation devices, channels and quantum key distribution protocols. The test of FOR QUANTUM COMPUTING COLLABORATION, UNIVERSITY OF ERLANGEN COLLABORATION — We present a method to test quantum behavior, HAUKE HASELER, TOBIAS MORODER, NORBERT LUTKENHAUS, Institute for Quantum Computing, INSTITUTE OF QUANTUM COMPUTING COLLABORATION, UNIVERSITY OF ERLANGEN COLLABORATION — We present a method to test quantum behavior of quantum information processing devices, such as quantum memories, teleportation devices, channels and quantum key distribution protocols. The test of quantum behavior can be phrased as the verification of effective entanglement. Necessary separability criteria are formulated in terms of a matrix of expectation values in conjunction with the partial transposition map. Our method is designed to reduce the resources for entanglement verification. A particular protocol based on coherent states and homodyne detection is used to illustrate the method. A possible test for the quantum nature of memories using two non-orthogonal signal states arises naturally. Furthermore, closer inspection of the measurement process in terms of the Stokes operators reveals a security threat for quantum key distribution involving phase reference beams.

11:27AM B15.00002 Testing Quantum Devices: Practical Entanglement Verification in Bipartite Optical Systems, HAUKE HASELER, TOBIAS MORODER, NORBERT LUTKENHAUS, Institute for Quantum Computing. INSTITUTE OF QUANTUM COMPUTING COLLABORATION, UNIVERSITY OF ERLANGEN COLLABORATION — We present a method to test quantum behavior of quantum information processing devices, such as quantum memories, teleportation devices, channels and quantum key distribution protocols. The test of quantum behavior can be phrased as the verification of effective entanglement. Necessary separability criteria are formulated in terms of a matrix of expectation values in conjunction with the partial transposition map. Our method is designed to reduce the resources for entanglement verification. A particular protocol based on coherent states and homodyne detection is used to illustrate the method. A possible test for the quantum nature of memories using two non-orthogonal signal states arises naturally. Furthermore, closer inspection of the measurement process in terms of the Stokes operators reveals a security threat for quantum key distribution involving phase reference beams.

11:39AM B15.00003 Transmission of photonic Bell states over a 2x32dB, 144km free-space link1, ALESSANDRO FEDRIZZI, R. URSIN, T. HERBST, M. NESPOLI, R. PREVEDEL, T. SCHEIDL, F. TIEFENBACHER, T. JENNENWEIN, IQOQI, Austrian Academy of Sciences, ANTON ZEILINGER, IQOQI; Faculty of Physics, University of Vienna — We successfully transmitted both photons of various Bell states over a 144 km free-space link between the islands of Tenerife and La Palma. Creating and transmitting more than $6 \times 10^9$ highly entangled photon pairs/s over the $2 \times 32$ dB channel we received 0.07 pairs/s at the receiver. We were able to distinguish between $|\psi^+\rangle$ and $|\psi^-\rangle$ states and verified the presence of entanglement by violating a CHSH Bell inequality to $S = 2.61 \pm 0.11$, 5 standard deviations above the classical limit of 2. Using a small and compact photon source, we effectively emulate quantum communication in a loss regime comparable to a two-link satellite communication scenario. Furthermore, we convincingly demonstrate the feasibility of 2-photon quantum communication protocols like dense coding, teleportation or quantum cryptography without reference frame over long distance. Finally, with a flight time of 0.5 ms the transmitted Bell states are the longest lived photonic Bell states ever reported.

1This work was supported by the Austrian Science Foundation (FWF), the Austrian Space Agency (FFG), the DTO funded U. S. Army Research Office and the City of Vienna.

11:51AM B15.00004 Correlated photon generation via four-wave mixing in a birefringent semiconductor waveguide, DANIEL ROGERS, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, JULIUS GOLDHAR, University of Maryland, CHRISTOPHER RICHARDSON, Laboratory for Physical Sciences, University of Maryland, ALESSANDRO RESTELLI, JOSHUA BIENFANG, CHARLES CLARK, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology — The next generation of quantum cryptography will benefit from a fast and practical source of entangled photon pairs. Current methods of generating entanglement, whether in bulk nonlinear crystals or microstructure optical fibers, pose significant challenges to integration into fieldable quantum communications systems. In order to meet the demands of speed and practicality, we investigate third-order nonlinearity in a semiconductor waveguide as a source of correlated and ultimately entangled photon pairs. This device offers an advantage over existing sources due to the relative ease of coupling to standard optical fibers. It is potentially useful for free-space and fiber-optic quantum key distribution as well as a host of other applications such as correlated photon metrology and two-photon interferometry. We show the feasibility of using phase-matched four-wave mixing in a birefringent AlGaAs waveguide to generate correlated photon pairs at wavelengths compatible with silicon detectors. We demonstrate the operation of such a device, consider the effects of loss and two-photon absorption, and evaluate the implications of birefringent phase matching.

12:03PM B15.00005 Macroscopic quantum memories get entangled from far away1, ZHEN-SHENG YUAN, YU-AO CHEN, SHUAI CHEN, JÖRG SCHMIEDMAYER, JIAN-WEI PAN, PHYSIKALISCHES INSTITUT, RUPEZRECHT-KARLS-UNIVERSITÄT HEIDELBERG, GERMANY TEAM, HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES, ATOMIC INSTITUT DER ÖSTERREICHISCHEN UNIVERSITÄTEN, TU-WIEN, AUSTRIA TEAM — We report an experimental implementation of a fundamental unit for long-distance quantum communication. By means of entanglement swapping, entanglement is generated between two remote atomic ensembles connected with either 6 m or 300 m fiber-based optical channel, where the flying qubits–two emitted photons from the atomic ensembles are sent to an intermediate station for a joint Bell-state measurement. Afterwards, the measurement induced entanglement between the atomic ensembles are verified by the violation of Bell’s inequality or by an entanglement witness. The striking features, phase-error insensitiveness and scalable flexibility, promise the present setup as a fundamental unit for future quantum information processing.

1This work was supported by the Deutsche Forschungsgemeinschaft (DFG), the Alexander von Humboldt Foundation, the Deutsche Telekom Stiftung the CAS.
12:15PM B15.00006 Long-distance atom-photon entanglement and its coherence properties. H. WEINFURTER, M. WEBER, J. VOLZ, W. ROSENFELD, M. KRUG, F. HOCKE, F. HENKEL, (1) SEKTION PHYSIK, LUDWIG-MAXIMILIANS-UNIVERSITY, D-80799 MUNICH, GERMANY COLLABORATION, (2) MAX-PLANCK-INSTITUTE FOR QUANTUM OPTICS, D-85748 GARCHING, GERMANY COLLABORATION — The distribution of entanglement between quantum memories at remote locations is one major challenge for the first demonstration of a quantum repeater. Entanglement between matter and light [1] is crucial for achieving this task. Here we report the observation of entanglement between a single trapped atom and a single photon, separated 300 m via an optical fiber. The entanglement is verified by appropriate correlation measurements of the atom-photon pair after communicating the photon through the fiber. In addition, we measure the temporal evolution of the atomic density matrix after projecting the atom-photon pair via a state measurement of the photon onto a well defined atomic spin state. We find that the atomic Zeeman qubit decoheres after 100 µs. Our results represent important steps towards the realization of entanglement between single neutral atoms at distances of several 100 m. [1] J. Volz, M. Weber, D. Schlenk et al., Phys. Rev. Lett. 96, 030404 (2006).

12:17PM B15.00007 Entanglement dynamics in a qubit-nanomechanical resonator system. DIAN WAHYU UTAMI, AASHISH CLERK, Physics Department, McGill University, Montreal — Over the recent years, finding signatures of entanglement in macroscopic systems has been a central goal in many aspects of mesoscopic physics. Here we present our study of non-equilibrium entanglement dynamics between a qubit and a nanomechanical resonator that is coupled to a phonon bath. Unlike previous studies, we specifically look at disspersive coupled qubit-oscillator system which has been realized in many different experiments. Using master equation expressed in gaussian wigner functions, we obtained an elegant and intuitive expression for the entanglement. Two ways of generating entanglement were found; entanglement of the qubit to the amplitude of the driven oscillator and to the phase of the oscillator. A full analytical result within the zero temperature limit of the two cases were derived. We also investigate the effect of finite temperature to the entanglement dynamics and found the phase entanglement to be more robust against temperature. The result indicates that an indirect method to measure the presence of entanglement in the system is possible.

12:19PM B15.00008 Generation of Entanglement Outside of the Light Cone. JAMES FRANSON, University of Maryland, Baltimore County — The probability amplitude to emit a photon at one location and then annihilate it at another location is proportional to the Feynman propagator, which has nonzero values outside of the forward light cone. This does not allow messages to be transmitted faster than light, but it does allow correlations, and mutual information to be generated outside the light cone. These effects are illustrated by considering two distant atoms, one of which is initially in its excited state and the other in its ground state. The probability amplitude for the two atoms to exchange a photon and make a transition to the other state is calculated using perturbation theory and commutator techniques, which gives a result proportional to the Feynman propagator. These effects can be interpreted as being due to the propagation of virtual photons outside of the light cone or as a transfer of pre-existing entanglement from the quantum vacuum.

12:21PM B15.00009 Towards single time-bin entangled photons from a quantum dot. CHRISTOPHE COUTEAU, GREGOR WEIHS, University of Waterloo — We present our results on photon statistics of quantum dots. We show evidence for photon antibunching and cross-correlation measurements within the biexciton-exciton cascade. We also discuss directions towards a demonstration of time-bin entangled photons from a dot. Recently, it has been showed theoretically that a quantum dot could provide pairs of time-bin entangled photons. The temporal entanglement is due to the fact that we know the twin photons will come in pairs but we don’t know when: either both the photons are really or both are late. Under the right conditions and using a double excitation of the dot corresponding to the two time bins, Simon and Poizat showed that one could get deterministic emission of pairs for time-bin entanglement using a single quantum dot. We present our latest results on photon statistics and our demonstration of photon antibunching as well as cross-correlations within the biexciton-exciton cascade using an original new set-up. Based on these measurements we are confident that we will be able to demonstrate time-bin entangled photons in the near future.

1:03PM B15.00010 Teleportation and Broadcasting of continuous variable entanglement. ARCHAN S. MAJUMDAR, SATYABRATA ADHIKARI, N. NAYAK, S. N. Bose National Centre for Basic Sciences — We present the first example for broadcasting of the entanglement of a two-mode squeezed state of the electromagnetic field shared by two distant parties into two nonlocal bipartite entangled states. Using the technique of covariance matrices we demonstrate the entanglement between the nonlocal output modes and the separability of the local output modes. We find the range of values for the squeezing parameter and the amplifier phase for which broadcasting of continuous variable entanglement can be implemented for physical states. We next present a scheme for teleporting two-mode entangled states of continuous variables from Alice to Bob. Our protocol is operationalized through the creation of a four-mode entangled state shared by Alice and Bob using linear amplifiers and beam splitters. Teleportation of the entangled state proceeds with local operations and the classical communication of four bits. We compute the fidelity of teleportation and find that it exhibits a trade-off with the magnitude of entanglement of the resultant teleported state. [arXiv:0708.1869; arXiv:0710.2777]

1:15PM B15.00011 Entanglement structure of two-mode squeezed states in absorbing and amplifying environment. PHOENIX S.Y. POON, C.K. LAW, Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, Hong Kong SAR, China — We examine the structure of entanglement for two-mode squeezed states interacting with symmetric linear baths [1]. In Fock space, $\rho^{TA}$ is observed to be maintaining a block diagonal form as the system evolves. We explicitly obtain the eigenvalues and eigenvectors of $\rho^{TA}$ (the partial transposition of density matrix $\rho$) as a function of time. The decoherence induced by the baths are shown to destroy the degeneracy of $\rho^{TA}$, leading to a set of eigenvectors for the construction of entanglement witness operators. We prove that the eigenvectors are time-independent, which is an indicator for the robustness of entanglement of two-mode squeezed states in the presence of noise. [1] Phoenix S. Y. Poon and C. K. Law, Phys. Rev. A 76, 012333 (2007).

1:27PM B15.00012 Quantum Second Law with Entanglement1. LADISLAV ANDREY, Academy of Sciences, Prague — It is proved rigorously that every quantum operation generating quantum entanglement states in the multipartite quantum system of qubits leads to the reduction of quantum entropy of whole system. By other words the quantum entanglement can be the source of quantum information. As the consequence the novel formulation of quantum second law is presented with possible applications to progressively developing quantum information science and quantum communications.

1:39PM B15.00013 Entanglement and Standard Thermodynamic Relations. INTI SODEMANN, University of South Carolina, ALONSO BOTERO, Universidad de Los Andes and University of South Carolina — We re-examine thermal properties of the standard (Boltzmann) canonical ensemble from the point of view of canonical typicality. In this approach, the thermodynamic system is described by the reduced density matrix of a correlated state from an energy-constrained total Hilbert space for the system and environment, with the entanglement entropy playing the role of thermodynamic entropy. We examine the average and variance of the entanglement entropy over all pure states of the restricted total Hilbert space, and show correspondence with the expected results of standard statistical mechanics in the limit of a large environment. We study the correlation between energy and entropy fluctuations, and show that the temperature can also be defined from a variational principle minimizing deviations from a microscopic version of the first law of thermodynamics, involving energy and entropy fluctuations.

This work was partly supported by the grant 1ET30010043 of GAAV and AVOZ 10300504.
Quantitative universality and non-local interactions in neural pattern formation. MATTHIAS KASCHUBE, Princeton University, MICHAEL SCHNABEL, MPI-DS, SIEGRID LOEWEL, University of Jena, DAVID COPPOLA, Randolph-Macon College, LEONARD WHITE, Duke University, FRED WOLF, MPI-DS — The occurrence of universal quantitative laws in a strongly interacting multi-component system indicates that its behavior can be elucidated through the identification of general mathematical principles rather than by the detailed characterization of its individual components. Here we demonstrate that universal quantitative laws govern the spatial layout of orientation selective neurons in the visual cortex in three mammalian species separated in evolution by more than 50 million years. Most suggestive of a mathematical structure underlying this universality, the average number of pinwheel centers per orientation hyper-column in all three species is statistically indistinguishable from the constant $\pi$. Mathematical models of neural pattern formation can reproduce all observed universal quantitative laws if non-local interactions are dominant, indicating that non-local interactions are constitutive in visual cortical development. The spatial layout adheres to these laws even if visual cortical organization exhibiting marked overall inhomogeneities and when neuronal response properties are experimentally altered. These results demonstrate that mathematical principles can shape the organization of the brain as powerfully as an organism's genetic make-up.

Spike-timing dependent plasticity in integrate-and-fire networks. CHUNG CHEN, DAVID JASON, University of Pittsburgh — We study plastic integrate-and-fire networks with spike-timing dependent plasticity. Following recent experiments, the long-term potentiation (depression) for causal (anti-causal) spike pairs is assumed to be additive (multiplicative) with reference to the existing synaptic strength. Assuming realistic physiological parameters, for time scales of minutes, the synaptic strength can be assumed fixed while neural activities equilibrate. A mean-field analysis in this regime predicts a first order phase transition for the neural activity. As the constant synaptic strength is increased, the network goes from a quiescent phase with only noise triggered activities, to a phase of persistent activity. The number of synapses per neuron controls the transition point in the synaptic strength. However, the activity level of the network just above the transition point is insensitive to the synapse number and represents a neural firing rate of about 20 to 30 Hz for the set of physiological parameters we considered. Simulations on random networks with fixed connectivities agree well with the mean-field predictions for a per-neuron synapse number of 10 or larger. Applying the plasticity rules and performing simulations covering physical times of days, at fixed depression factor for anti-causal spike pairs, the networks develop a unimodal distribution of synaptic strengths at small potentiation values for causal pairs, while run-away synaptic strengths are observed at large values.

A Maximum Entropy Model Applied to Temporal Correlations in Cortical Networks. WEI CHEN, AONAN TANG, JON HOBBS, JODI L. SMITH, HEMA PATEL, ANITA PRIETO, JOHN BEGGS, Indiana University, DAVID JACKSON, Brown University, DUMITRU PETRUSCA, MATTHEW I. GRIVICH, ALEXANDER SHER, ALAN M. LITKE, University of California, Santa Cruz — Multi-neuron firing states are often observed, yet are predicted to be rare by models that assume independent firing. To predict these states, two groups recently applied a second-order maximum entropy model that used only observed firing rates and pairwise interactions as parameters (Schneidman et al., 2006; Shin et al., 2006). Interestingly, these models predicted 90-99% of network correlations. If generally applicable, this approach could vastly simplify analyses of complex networks. However, this work did not address the temporal evolution of correlated states. We applied the model to multielectrode data from cortical slices and cultures. In 8/13 preparations the observed sequences of correlated states were significantly longer than predicted by concatenating states from the model. We found a significant relationship between strong pairwise temporal correlations and observed sequence length, suggesting that pairwise temporal correlations may allow the model to be extended into the temporal domain.

Effective connectivity in a network of spiking cortical neurons. AONAN TANG, JON HOBBS, WEI CHEN, Indiana University, DUMITRU PETRUSCA, MATTHEW GRIVICH, ALEXANDER SHER, ALAN LITKE, University of California, Santa Cruz, JOHN BEGGS, Indiana University — The average cortical neuron makes and receives about 1,000 synaptic contacts. This anatomical information suggests that local cortical networks are connected in a fairly democratic manner, with all nodes having about the same degree. But the physical connections found in the brain do not necessarily reveal how information flows through the network. We used transfer entropy (Schreiber, 2000) to assess effective connectivity in cortical slice cultures placed on a 512 electrode array system (in collaboration with Alan Litke of UC Santa Cruz). These cultures ($n = 6$) were active for periods exceeding 1 hr, allowing us to collect long data sets for entropy statistics. Data were binned at 1 ms to match the width of a single neural spike. Analysis revealed widespread differences in node degrees, but did not clearly point to a small-world or a scale-free structure.

Inhibition is Needed to Learn Precise Multimodal Integration$^1$. J. LEO VAN HEMMEN, Physik Department, TU Munich — Multimodal neuronal maps, combining input from two or more sensory systems, e.g., vision and audition, play a key role in processing and transforming sensory to motor information. For such maps to be of any use, the input from all participating modalities must be calibrated so that a stimulus at a specific spatial location is represented at an unambiguous position in the multimodal map. Here we discuss a method based on supervised spike-timing-dependent plasticity (STDP) to gauge input from different sensory modalities so as to ensure proper map alignment. We therefore analyze excitation- and inhibition-mediated learning in conjunction with the problem of how perfect a teacher should be. Analytical calculations and numerical simulations show on the one hand that inhibitory teacher input is essential if high-quality multimodal integration must be learnt rapidly. On the other hand, the quality of the resulting map is not limited by the quality of the teacher signal alone but rather by the accuracy of the input from other sensory modalities.

Distinguishing Similar Odor Stimuli in Nonlinear Recurrent Networks. STUART WICK, Northwestern U, MARTIN WIECHERT, RAINER FRIEDRICH, Friedrich Miescher Inst., Basel, HERMANN RIECKE, Northwestern U — The olfactory bulb (OB) is the first processing stage for olfactory information and receives input in the form of activity patterns across an array of discrete input channels (glomeruli). Experiments show that the OB decorrelates similar olfactory inputs: the output patterns are more distinct than the input patterns, which is likely to be important for downstream computations. The high dimensionality of odor space implies a fractured representation of odors on the two-dimensional array of glomeruli. The neural circuits achieving the decorrelation must therefore be non-trivial; their connectivity is, however, poorly known. We investigate what connectivities are optimally suited for this task. For neural networks with linear dynamics the connectivity can be given explicitly. Experiments indicate, however, that the bulbar dynamics are strongly nonlinear and must be minimally modeled by a piece-wise linear rectifier. We investigate the impact of the rectifier on two types of connectivities which are optimal for linear networks, but only one of which accomodates the rectifier. We test the performance of both types of networks by adapting them to an ensemble of odors and assessing their ability to decorrelate these and related odors at the same and other concentrations.
12:27PM B16.00007 A low dimensional description of globally coupled heterogeneous neural networks of excitatory and inhibitory neurons. ROXANA A. STEFANESCU, Florida Atlantic University, VIKTOR K. JIRSA, CNRS and Florida Atlantic University — Neural networks consisting of globally coupled excitatory and inhibitory non-identical neurons may exhibit a complex dynamic behavior including synchronization, multi-clustered solutions in phase space and oscillator death. We investigate the conditions under which these behaviors occur in a multidimensional parametric space defined by the connectivity strengths and dispersion of the neuronal membrane excitability. Using mode decomposition techniques, we further derive analytically a low dimensional description of the neural population dynamics and show that the dynamics of the entire network can be very well reproduced by this reduced system. Examples of networks of FitzHugh-Nagumo and Hindmarsh-Rose neurons are discussed in detail.

12:39PM B16.00008 A Neuron-Based Model of Sleep-Wake Cycles. SVETLANA POSTNOVA, University of Marburg, ACHIM PETERS, University of Luebeck, HANS BRAUN, University of Marburg — In recent years it was discovered that a neuropeptide orexin/hypocretin plays a main role in sleep processes. This peptide is produced by the neurons in the lateral hypothalamus, which project to almost all brain areas. We present a computational model of sleep-wake cycles, which is based on the Hodgkin-Huxley type neurons and considers reciprocal glutameric projections between the lateral hypothalamus and the prefrontal cortex. Orexin is released as a neuromodulator and is required to keep the neurons firing, which corresponds to the wake state. When orexin is depleted the neurons are getting silent as observed in the sleep state. They can be reactivated by the circadian signal from the suprachiasmatic nucleus and/or external stimuli (alarm clock). Orexin projections to the thalamocortical neurons also can account for their transition from tonic firing activity during wakefulness to synchronized burst discharges during sleep.

1 Supported by the EU Network of Excellence BioSim No. LSHB-CT-2004-005137

12:51PM B16.00009 Interdependencies of Neural Impulse Pattern and Synchronization. HANS BRAUN, SVETLANA POSTNOVA, HORST SCHNEIDER, University of Marburg — Neuronal synchronization plays a crucial role in many physiological functions such as information binding and wake-sleep transitions as well as in pathophysiological processes like Parkinson’s disease and epileptic seizures. The occurrence of synchronized activity is often associated with significant alterations of the neuronal impulse pattern, mostly with a transition from tonic firing to burst discharges. We have used Hodgkin-Huxley type simulations to study how alterations of individual neurons’ dynamics influence the synchronization in electrotonically coupled networks. The individual neurons have been tuned from tonic firing to bursting with chaotic dynamics in between. Our results demonstrate that these transitions have significant impact on the neurons’ synchronization. Vice versa, the synchronization state can essentially modify the impulse pattern. The most remarkably effects appear when the individual neurons operate in a periodically tonic firing regime close to the transition to chaos.

1 Supported by the EU through the Network of Excellence BioSim, Contract No. LSHB-CT-2004-005137.

1:03PM B16.00010 Mosaics of retinal cells that transmit maximal information. TATYANA SHARPEE. The Salk Institute for Biological Studies — In the nervous system, visual signals are encoded by retinal ganglion cells into sequences of discrete electrical pulses termed spikes. Response properties of different ganglion cell types are encoded visual field and are arranged on approximately hexagonal lattice. Here we consider the optimal arrangement of response regions that would collectively allow for maximal information transmitted about the location of a point light source. We find that maximal information can be transmitted when at most three neighboring regions overlap and the average radius of response field is ~0.67 of the distance between response field centers. This finding was obtained with no adjustable parameters and agrees with experimental measurements of retinal mosaics [1, 2].


1:15PM B16.00011 Phase synchronization analysis of voltage-sensitive dye imaging during drug-induced epileptic seizures. DAISUKE TAKESHITA, VASSILY TSYTSAREV, SONYA BAHAR, Dept. of Physics and Astronomy and Center for Neurodynamics, University of Missouri-St. Louis — Epileptic seizures are generally held to result from excess and synchronized neural activity. However, recent studies have suggested that this is not necessarily the case. We investigate how the spatiotemporal pattern of synchronization changes during drug-induced in vivo neocortical seizures in rats. Epileptic seizures are caused by the potassium channel blocker 4-aminopyridine, which is often used in experiments to induce epileptic seizures. In our experiments, the neocortex is stained with the voltage-sensitive dye RH-1091. The intensity changes in dye fluorescence are measured by a CCD camera and are consistent with the signal from local field potential recording. We apply phase synchronization analysis to the voltage-sensitive dye signals from pairs of pixels in order to investigate the degree to which synchronization occurs, and how spatial patterns of synchrony may change, during the course of the seizure. Our preliminary results show that two distant pixels are well synchronized during a seizure event.

1:27PM B16.00012 Information transfer in ampullary electroreceptors. ALEXANDER NEIMAN, Ohio University, TATIANA ENGEL, Max Planck Institute of Colloids and Interfaces — Many neurons in central nervous system and in sensory periphery are characterized by significant correlations between consequent interspike intervals of their stochastic spontaneous activity. Such non-renewal stochastic dynamics can result from internal properties of a neuron, such as spike-frequency adaptation, as well as from external perturbations or both. We consider one example of such system, peripheral ampullary electroreceptors in paddlefish. Spontaneous dynamics of electroreceptors is characterized by extended serial correlations of interspike intervals resulting from nonlinear interaction of two stochastic oscillators embedded into the system. Using computational modeling and approaches from information theory we show that these correlations significantly improve information transfer of weak external stimuli.

[1] Supported by NIH grant DC04922 to D.F. Russell

1:39PM B16.00013 Spike-time-variability in stochastic Hodgkin-Huxley type neural models. PETER ROWAT, University of California San Diego — When the classical Hodgkin-Huxley equations are simulated with Na- and K-channel noise and fixed applied current, the distribution of inter-spike intervals is bi-modal: one part is an exponential tail, as often assumed, while the other is a narrow gaussian peak centered at a short ISI value. The gaussian arises from bursts of spikes in the gamma-frequency range, the tail from the inter-burst-intervals, giving overall a very high coefficient of variation: up to 2.5 for 180,000 Na-channels. Since neurons with a bimodal inter-spike interval distribution are common, it may be a useful model for any neuron with class 2 firing. The underlying mechanism is due to a sub-critical Hopf bifurcation together with a switching region in phase-space where a fixed point is very close to a system limit cycle. This mechanism may contribute to highly irregular spike times in cortex. Other mechanisms underlying neural variability will also be presented.
activity with increased/decreased number of spikes per burst. The neural bursts and Ca\(^{2+}\) connection strengths. In the neural networks with "all-with-all" connections and AMPA/GABA synapses an increase in average synaptic strength yielded bursting activity with increased/decreased number of spikes per burst. The neural bursts and Ca\(^{2+}\) transients were synchronous at relatively large connection strengths despite random connection strengths. Simulations of the neural networks with 20 connections per neuron and with only AMPA synapses showed synchronous oscillations, while the neural networks with GABA or hybrid synapses generated propagating waves of membrane potential and Ca\(^{2+}\) transients.

1:27AM B17.00002 Adhesion induces and localizes phase separation in lipid membranes. MARKUS DESERNO, Carnegie Mellon University, VERNITA GORDON, University of Illinois, Urbana-Champaign, CAROLINE ANDREW, University of Edinburgh — We study the evolution of GUVs from spherical to pearl-like and to tube-like shapes, and back again reversibly.

1:39AM B17.00003 Cholesterol Effect on Phase Behavior in Ternary Lipid Membrane—X-ray Diffraction and AFM. JING YUAN, ALEX KISS, YOHANES PRAMUDYA, LAM NGUYEN, LINDA HIRST — There is growing evidence that lipid membranes are not uniform, but contain lipid microdomains or "rafts", which are enriched in cholesterol, saturated long-chained lipids, and particular proteins. The effects of cholesterol on lipid ordering and phase separation in lipid-rafts-contained model membrane systems have been investigated by Synchrotron X-ray Diffraction and Atomic Force Microscope (AFM). We have measured bilayer d-spacings in two ternary lipid mixtures: DOPC/eSM/Cholesterol and DOPC/DPPC/Cholesterol, as cholesterol content is varied. Mixtures containing intermediate amounts of cholesterol exhibited two phases, and for DOPC/eSM/Cholesterol with 10% and 12% cholesterol, three d-spacings were observed, indicating the possible coexistence of three different phases: liquid disordered (ld) phase, liquid ordered (lo) phase, and gel phase. AFM images of supported lipid bilayers on mica substrates contained clearly visible raft-like micro-domains in the similar cholesterol amount range.

1This work is supported by the MARTECH and the Institute of Molecular Biophysics, both at Florida State University.

11:51AM B17.00004 Thermodynamic properties of planar membranes: applications to stripped phases. FRANCISCO J. SOLIS, Integrated Natural Sciences, Arizona State University, CHLOE FUNKHAUSER, KATSUYO THORNTON, Materials Science and Engineering, University of Michigan — Multicomponent membranes can have shapes that are planar at large length scales while retaining complex morphologies at smaller scales. We explore the properties of these membranes that arise from the planarity condition. We show that planarity requires that the average stress tensor of the membrane be parallel to the planar directions. We apply this description of planar membranes to the case of lipid bilayers.

12:03PM B17.00005 Phospholipid Membranes Restructure Locally Where Nanoparticles Bind, BO WANG, YAN YU, STEPHEN ANTHONY, SUNG CHUL BAE, STEVE GRANICK, University of Illinois — In the field of surface science, it is known that metal and semiconductor surfaces may respond to their environment by restructuring. Similar issues are more significant in nanoscience, since large populations of the atoms/molecules reside on the surfaces. It is natural to inquire whether analogous restructuring might also be characteristic of phospholipid membranes, bearing mind that no bulk exists at all in this case. We show here that the two categories of reconstructions, phase state and local curvature, of unicomponent lipid bilayers can occur through non-specific interactions when charged nanoparticles adsorb. This coupling not only modulates the short-range molecular orientation and packing, but also is believed to be responsible for long-range interaction and transportation on fluctuating membranes.

12:15PM B17.00006 Multiscale Modeling of supported lipid bilayers, ROLAND FALLER, CHENYUE XING, MATTHEW HOOPES, UC Davis — The study of lipid structure and phase behavior at the nano scale length is of importance due to implications in understanding the role of the lipids in biochemical membrane processes. We performed a variety of simulations in homogeneous and heterogeneous membrane systems to elucidate such behaviors. Our simulations demonstrate that various coarse grained simulation models can predict different aspects of lipid phase separation and describe the change of the system under the influence of a support. The simulations are performed using models at different length scales ranging from the atom scale to a scale where lipids are modeled by only three interaction sites. We are able to follow transformations, such as lipid phase transitions. These phase transitions are determined by analyzing parameters like area per lipid head group, the deuterium order parameter and dynamic properties. Additionally, we characterize individual lipid molecules using rotational correlation functions to classify different dynamic populations and we study the stability of artificially designed patterns. We discuss the changes of the system phase behavior as well as differences between the two leaflets as induced by the support.
12:27PM B17.00007 Synergy of Membrane Curvature-Stabilization and Electrostatic Interaction leads to Formation of Block Liposomes by Colossal Charged Lipids, ALEXANDRA ZIDOVSKA, KAI K. EWERT, CYRUS R. SAFINAYA, Materials, Physics, and Molecular, Cellular and Developmental Biology Departments, University of California, Santa Barbara, JOEL QUISPE, BRIDGET CARRAGHER, CLINTON S. POTTER, National Resource for Automated Molecular Microscopy, The Scripps Research Institute, La Jolla — Recently, we have reported block liposomes (BLs), a new vesicle phase formed in mixtures of MVLB2G, DOPC and water (A. Zidovska et al., Submitted, 2007), where MVLB2G is a newly synthesized highly charged (16+) lipid (K. Ewert et al., JACS, 2006) with giant dendrimer-like headgroup. BLs are liposomes consisting of distinctly shaped nanoscale spheres, pears, tubes, or rods connected into blocks. In this work we investigate the contribution of spontaneous curvature and membrane charge density to the formation of BLs. By comparing with a system of matching membrane charge density but zero spontaneous curvature and by screening the charge of MVLB2G but keeping the curvature constant, we were able to identify both, spontaneous curvature and membrane charge, as critical parameters for BLs-formation. The effect of salt and pH on the shape evolution of the BLs was also carefully studied. Funding provided by DOE DE-FG-02-06ER46314, NIH GM-59288, NSF DMR-0503347.

12:39PM B17.00008 Photo-induced Phase Separation Phenomena in Lipid Tubules, LINDA HIRST, JING YUAN, Florida State University — The self-assembly of biological amphiphiles has proved a fascinating topic in recent years, the hollow cylindrical lipid tubule morphology being of particular interest due to its potential relevance to intercellular transporting channels and applicability to controlled-release systems, chemical micro-reactors and nano-conductors. Co-existence of the liquid-ordered and liquid-disordered phases in the lipid bilayer has recently been observed in biologically-relevant three-component giant unilamellar vesicles. We have generated stable, photo-induced micron-scale phase separation in lipid tubules formed from ternary lipid mixtures, inducing a new bilayer disc structure. This investigation not only aids in our understanding of lipid sorting phenomena in cell membranes (suggesting a mechanism for bilayer disc formation in retinal rod-cells), but is also a fascinating route to the generation of new, functional structures. This work is supported by the MARTECH and the Institute of Molecular Biophysics, both at Florida State University.

12:51PM B17.00009 Dynamics of Multi-Component Model Membranes Studied via Light and X-Ray Scattering, KEVIN JOHNSON, MAIKEL RHEINSTÄDTGER, University of Missouri — We study the dynamics of multicomponent biological model membranes (phospholipid, ethanol, cholesterol systems) via X-ray and light scattering to probe the dynamics of such membranes in solid supported and freestanding configurations. Collective molecular motions may play a significant role in different biological functions such as transmembrane transport and pore opening processes. Our main research objective is to quantify collective molecular motions in membranes and establish relationships to key physiological and biological functions of the bilayers. The phase diagram of this system with varying cholesterol and ethanol concentrations at set temperatures is determined using X-ray diffraction techniques and the mesoscopic membrane dynamics is then measured using time correlation light scattering techniques. The results can be compared to molecular dynamics simulations in a coarse grained membrane model. The dynamics shows propagating and relaxing processes, which allow to determine, e.g. the elasticity parameters of the bilayers. By understanding the mesoscopic properties of membranes with selected composition, membranes with specific properties can be designed.

1:03PM B17.00010 The Impact of Collective Molecular Dynamics on Physiological and Biological Functionalities of Artificial and Biological Membranes, MAIKEL RHEINSTÄDTGER, University of Missouri-Columbia — We use neutron, X-ray and light scattering techniques to determine dynamical and structural properties of artificial and biological membranes. The combination of various techniques enlarges the window to length scales from the nearest-neighbor distances of lipid molecules to more than 10^{-6} m, covering time scales from about 0.1 ps to 1 s. The main research objective is to quantify collective molecular fluctuations in these systems and to establish relationships to physiological and biological functions of the bilayers, such as transmembrane transport. The motivation for this project is twofold: 1) By understanding fundamental properties of bilayers at the microscopic and mesoscopic level, we aim to tailor membranes with specific properties such as permeability and elasticity. 2) By relating dynamical fluctuations to physiological and biological functions, we can gain a deeper understanding of the bilayers on a molecular scale that may help optimizing the transmembrane transport of certain drugs. We show how bilayer permeability, elasticity and inter protein excitations can be determined from the experiments. M.C. Rheinstädter et al., Phys. Rev. Lett. 93, 108107 (2004); Phys. Rev. Lett. 97, 048103 (2006); Phys. Rev. E 75, 011907 (2007); J. Vac. Soc. Technol. A 24, 1191 (2006).

1:15PM B17.00011 ABSTRACT WITHDRAWN —

1:27PM B17.00012 Effect of anesthetics on bending elasticity of lipid membranes, ZHENG YI, Indiana University, NAGAO MICHIIHO, NIST/Indiana University, DOBRIN BOSSEV, Indiana University — Change in physical and chemical properties of bio-membranes is of great interest for understanding the mechanism of anesthetic action on membranes. Hypothetically the anesthetic alters the lipid membrane structure (promoting pore formation across membranes or at least switching transmembrane channels) and therefore the biophysical properties of the membrane. We have used neutron spin echo (NSE) spectroscopy to study the effect of anesthetic molecule, lidocaine, on the bending elasticity (BE) of lipid membranes. BE of lipid bilayers made of (1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine) DMPC and 1,2-Dipalmitoyl-sn-Glycero-3-Phosphocholine (DPPC) have been measured at different temperatures and different in the fluid (L_{alpha}) phase. Using Zilman-Granek theory the BE were obtained from the decay of the NSE intermediate scattering function. We have found that in the presence of lidocaine the BE of DMPC and DPPC bilayers increases. The results were correlated with those from differential scanning calorimetry. Increase in the lidocaine concentration leads to decrease in the liquid/crystalline transition temperature.

1:39PM B17.00013 Interactions between non-steroidal anti-inflammatory drugs and lipid membranes, MOHAN BOGGARA, RAMANAN KRISHNAMOORTI, Dept of Chemical and Biomolecular Enng, Univ of Houston — Chronic usage of Non-steroidal anti-inflammatory drugs(NSAIDs) leads to gastrointestinal toxicity and clinical evidences point the cause to direct interactions between NSAIDs and phospholipid membranes. Also, NSAIDs pre-associated with phospholipid vesicles are shown to be safer and therapeutically more effective than unmodified ones. Our initial experiments and simulations on the partitioning of Aspirin and Ibufrofen clearly indicate role played by the drug structure in drug-membrane interactions. Those results motivated systematic molecular dynamics simulations of membranes with NSAIDs of different size, structure and pKa values. Our results suggest high partition coefficients for these NSAIDs in the membrane compared to water and thinning effect on the bilayer. Our small angle neutron scattering and reflectivity studies on DMPC-Ibufrofen systems indicate that the drug affects both ~5 nm thick bilayer and overall ~100 nm diameter vesicle, indicating that NSAIDs affect vesicles on various length scales. We will discuss the structural perturbations to membranes due to NSAIDs at clinically relevant molar ratios and their implications on the use of vesicles as delivery vehicles for NSAIDs.1

NIST Center for Neutron Research is duly acknowledged.

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1:39PM B17.00013 Interactions between non-steroidal anti-inflammatory drugs and lipid membranes, MOHAN BOGGARA, RAMANAN KRISHNAMOORTI, Dept of Chemical and Biomolecular Enng, Univ of Houston — Chronic usage of Non-steroidal anti-inflammatory drugs(NSAIDs) leads to gastrointestinal toxicity and clinical evidences point the cause to direct interactions between NSAIDs and phospholipid membranes. Also, NSAIDs pre-associated with phospholipid vesicles are shown to be safer and therapeutically more effective than unmodified ones. Our initial experiments and simulations on the partitioning of Aspirin and Ibufrofen clearly indicate role played by the drug structure in drug-membrane interactions. Those results motivated systematic molecular dynamics simulations of membranes with NSAIDs of different size, structure and pKa values. Our results suggest high partition coefficients for these NSAIDs in the membrane compared to water and thinning effect on the bilayer. Our small angle neutron scattering and reflectivity studies on DMPC-Ibufrofen systems indicate that the drug affects both ~5 nm thick bilayer and overall ~100 nm diameter vesicle, indicating that NSAIDs affect vesicles on various length scales. We will discuss the structural perturbations to membranes due to NSAIDs at clinically relevant molar ratios and their implications on the use of vesicles as delivery vehicles for NSAIDs.

1 NIST Center for Neutron Research is duly acknowledged.
1:51PM B17.00014 Calorimetric and Optical Studies of Cholesterol-Rich Filamentous, Helical Ribbon, and Crystal Microstructures, KLaida Kashuri, Germano S. Iannacchione, Worcester Polytechnic Institute (WPI), Yekaterina A. Miroshnikova, Yevgeniya V. Zastavker, Franklin W. Olin College of Engineering, Worcester Polytechnic Institute (WPI) Team, Franklin W. Olin College of Engineering Team — Calorimetry (differential-scanning and modulation) and optical phase contrast microscopy studies have been performed on the filamentous, helical ribbon, and crystal microstructures formed in Chemically Defined Lipid Concentrate (CDLC). CDLC is a quaternary sterol system consisting of a cholesterol, bilayer-forming amphiphiles, micelle-forming amphiphiles, and water. Phase contrast microscopy confirms the presence of the three microstructure types in all samples studied. Sample size and temperature scan rate were varied on samples ranging from 1 to 20 mg and rates from 0:017 to 1 degree C/min, respectively. Thermal profiles are strongly dependent on sample size, scan rate, and thermal history. These scans also reveal numerous “transition” features, likely due to melting of various microstructures in CDLC, that generally shift to higher temperatures with increasing sample size. These results indicate that the filamentous, helical ribbon, and crystal microstructures formed in CDLC may be coexisting in a meta-stable chemical equilibrium with each other and the solvent environment from which they grow.

2:03PM B17.00015 Structural and dynamical properties of water at the bilayer DPPC membrane interface, Jianping Gao, Charles Cleveland, Uzi Landman, School of Physics, Georgia Institute of Technology — The properties of interfacial water near the DPPC lipid bilayer surface are probed by a nano-size quartz tip through large scale atomistic molecular dynamics simulations. The water films confined between the bilayer membrane surface and a crystalline wetting quartz surface are kept in contact with a water reservoir at 293K. The distance between the solid tip and the gel phase membrane is varied between 0.5 to 2 nanometers. Layering of the confined water film is found near the solid tip while the water at the membrane surface remains unlayered. Some water is trapped in the cavities between the head groups of the lipid molecules. The recorded solvation force does not show oscillations due to the rough nature of the membrane surface.


11:15AM B18.00001 High Strain Deformation and Fracture of Self-Assembled Polymer Gels, Kenneth Shull, Northwestern University — Triblock copolymers with poly(methyl methacrylate) (PMMA) endblocks and a poly(n-butyl acrylate) (PNBA) midblock form thermoreversible gels in a variety of alcohols. The mechanical response of the gels is determined by the nature of the PMMA aggregates that are bridged by PNBA midblocks. The close proximity of the ordering temperature to the glass transition of the PMMA aggregates gives rise to a remarkably strong temperature dependence of the relaxation time for the polymer gels. At low temperatures, where the relaxation times are very large, the gels can be deformed to very large strains prior to solid-like fracture. At intermediate temperatures the materials flow, but strain localization leads to a melt fracture phenomenon, and at higher temperatures the materials behave as viscous polymer solutions. We have used these gels as a model material for studying rate effects in the high strain deformation and fracture of soft solids.

11:51AM B18.00002 Reinforcement of Epoxies Using Single Walled Carbon Nanotubes, Ramanan Krishnamoorti, Jitendra Sharma, Tirtha Chatterjee, University of Houston — The reinforcement of bisphenol-A and bisphenol-F epoxies using single walled carbon nanotubes has been approached experimentally by understanding the nature of interactions between the matrices and nanotubes. Unassisted dispersions of single walled carbon nanotubes in epoxies were studied by a combination of radiation scattering (elastic small angle scattering and inelastic scattering), DSC based glass transition determination, melt rheology and solid-state mechanical testing in order to understand and correlate changes in local and global dynamics to the tailoring of composite mechanical properties. Significant changes in the glass transition temperature of the matrix can successfully account for changes in the viscoelastic properties of the epoxy dispersions for concentrations below the percolation threshold, while above the percolation threshold the network superstructure formed by the nanotubes controls the viscoelastic properties.

12:03PM B18.00003 Mechanical and Electrical Properties of Organogels with Multiwall Carbon Nanotubes, Mohammad Moniruzzaman, Karen Winey, University of Pennsylvania — Organogels are fascinating thermally reversible viscoelastic materials that are composed of an organic liquid and low concentrations (typically <2 wt %) of low molecular mass organic gelators. We have fabricated the first organogel/carbon nanotube composites using 12-hydroxystearic acid (HSA) as the gelator molecule and pristine and carboxylated multi-wall carbon nanotubes as the nanofillers and 1,2-dichlorobenzene as the organic solvent. We have achieved significant improvements in the mechanical and electrical properties of organogels by incorporating these carbon nanotubes. For example, the linear viscoelastic regime of the HSA organogel, an indicator of the strength of the gel, extends by a factor of 4 with the incorporation of 0.2 wt% of the carboxylated nanotubes. Also, the carbon nanotubes (specially the pristine tubes) improve the electrical conductivity of the organogels, e.g. six orders of magnitude enhancement in electrical conductivity with 0.2 wt% of pristine tubes. Differential scanning calorimetry experiments indicate that the nanotubes do not affect the thermoreversibility of the organogels.

12:15PM B18.00004 Identification of key deformation mechanisms of polyethylene materials via in-situ x-ray scattering, Theresa Hermel-Davidock, Brian Landes, Mehmet Demirors, The Dow Chemical Company — Changes in the microstructure of ethylene based copolymers can be used to modify and enhance their mechanical performance. In this study, the effects of comonomer content, molecular weight, and molecular weight distribution on the mechanical performance of select polyethylene polymers were examined. Two key performance parameters for commercial polymer materials, especially in the area of blown film applications, are tear resistance and puncture resistance. However, polyethylene films which exhibit very similar morphology often exhibit very different Dart and Elmendorf tear values which cannot be differentiated by standard tensile test methods. Alternative methods to link morphology and mechanical response need to be found. Wide-angle and small-angle x-ray scattering was collected during in-situ tensile testing to understand how compositional and structural differences affect the mechanical response of semicrystalline polyethylene polymers. Microstructural changes observed during the in-situ deformation process are correlated to Elmendorf tear performance for both intrinsic and blown film samples.
12:27PM B18.00005 Brittle-tough transitions during crack growth in toughened adhesives
MICHAEL THOULES, University of Michigan — The use of structural adhesives in automotive applications relies on an effective understanding of their performance under crash conditions. In particular, there is considerable potential for mechanics-based modeling of the interaction between an adhesive layer and the adherends, to replace current empirical approaches to design. Since energy dissipation during a crash, mediated by plastic deformation of the structure, is a primary consideration for automotive applications, traditional approaches of fracture mechanics are not appropriate. Cohesive-zone models that use two fracture parameters - cohesive strength and toughness - have been shown to provide a method for quantitative mechanics analysis. Combined numerical and experimental techniques have been developed to deduce the toughness and strength parameters of adhesive layers, allowing qualitative modeling of the performance of adhesive joints. These techniques have been used to study the failure of joints, formed from a toughened adhesive and sheet metal, over a wide range of loading rates. Two fracture modes are observed: quasi-static crack growth and dynamic crack growth. The quasi-static crack growth is associated with a toughness of the adhesive. Generic, the work done by the applied force on the fracture opening area per unit crack extension length is proportional to the energy dissipated. The results of the experiments indicate that the fracture parameters for quasi-static crack growth in this toughened system are essentially rate independent, and that quasi-static crack growth can occur even at the highest crack velocities. Effects of rate appear to be limited to the ease with which a transition to dynamic fracture could be triggered. This transition appears to be stochastic in nature, and it does not appear to be associated with the attainment of any critical value for crack velocity or loading rate. Fracture mechanics failures do exist in the literature for brittle-ductile transitions in rate-dependent polymers, which rely on rate dependent values of toughness with unstable branches. The present observations do not appear to follow the type of behavior that would be expected from these models, but are consistent with prior observations of fracture instabilities in bulk polymer rubber-toughened epoxies. Some alternative models for the transitions in fracture mode will be discussed.

1:03PM B18.00006 Controlling polymer adhesion with surface wrinkles, EDWIN CHAN, Massachusetts Institute of Technology, ERICA SMITH, Trinity College, RYAN HAYWARD, ALFRED CROSBY, University of Massachusetts Amherst — One of nature’s solutions in controlling adhesion is through the intelligent design of patterned interfaces. For example, the feet of geckos and some insects are decorated with fibrillar structures designed specifically for locomotion, i.e. enhanced control of adhesion and release. Recently, there have been significant efforts in mimicking these materials to develop synthetic analogs to tailor polymer adhesion. However, challenges such as reusability and fabrication scalability limit the successful applications of these materials. In this work, we present an alternative approach to the design of a patterned adhesive that utilizes surface wrinkles to control the adhesion of a polymer (n-butyl acrylate) (PnBA) elastomer. Using a probe-type contact adhesion test, we experimentally show that surface wrinkles enhance adhesion of the PnBA elastomer based on a mechanism termed contact line splitting. We demonstrate that the efficiency of this contact line splitting mechanism is coupled with the wavelength of the wrinkles. Furthermore, the geometry of the surface wrinkles facilitates a repeatable interfacial response necessary to function as a reusable adhesive. Our approach provides a simple and scalable strategy to the design of patterned adhesives that is amenable to a variety of polymeric materials while facilitating enhanced control of interfacial response.

1:15PM B18.00007 Soft-soft nanocomposite adhesives made from colloidal particles, COSTANTINO CRETON, FANNY DEPLACE, ESPCI, MICHAEL RABJOHNS, ANDREW FOSTER, PETER LOVELL, University of Manchester, CHUNGHONG LEI, JOSEPH KEOUIE, University of Sheffield, SERGEY PANYUKOV, P.N. Lebedev Physics Institute, Russian Academy of Sciences, Moscow, Russian Federation, MICHAEL LANG, Leibniz-Institute for Polymer Research, Hohe Str, 6, 01069 Dresden, Germany — We investigate ideal Gaussian networks both analytically and with computer simulations using the Bond Fluctuation model with and without excluded volume interactions. The focus of this study is on fluctuations and the collapse of networks with different connectivity and dimensionality. We show that the size of a perfect square 2D network made from $N^2$ Gaussian chains with $N$ monomers each is $R_g \sim N^{1/2} \log(n)$. Thus fluctuations in two-dimensional networks diverge logarithmically with the size of these films while fluctuations of three-dimensional networks $\sim N^{3/2}$ and do not increase with their size. We study the cross-over between two and three-dimensional networks by following the dependence of junction fluctuations on the thickness of films. The results of model systems are compared with more realistic networks in order to understand the effect of disorder on the properties of the network and fluctuations of network junctions.

1:27PM B18.00008 Dangling chain effect on the modulus of polyurethane networks, BRUNO FAYOLLE, JULIE DIANI, PIERRE GILORMINI, Arts et Métiers ParisTech — While the theory of elasticity has been well verified for the non ideal structures accounting for contribution of entanglements, some effort is needed to investigate the contribution of dangling chains. In order to establish a quantitative contribution of dangling chains, networks with a controlled architecture, i.e. where architecture is determined by synthesis of well-characterized reactants, are required. In this work, polyurethane networks based on (poly(propylether) and poly(tetramethyl adipate) crosslinked by triisocyanate were prepared and studied. Different polyether molar masses are chosen from 430 g/mol up to 4000 g/mol. By varying the stoechiometric ratio $r = [\text{NCO}] / [\text{OH}]$ between 0.4 and 1, dangling chains are introduced, provided that the reaction between NCO groups is negligible. After synthesis, the Young’s modulus (E) of the networks has been measured from tensile tests according to the neo-Hookean law. The molar mass of elastically active network chains (ENAC) is determined from E. Since this molar mass is close to the molar mass of each diol used for synthesis at $r=1$ ("ideal" network), a correction taking into account the number of dangling chains (b) calculated from r is proposed.

1:39PM B18.00009 Morphological Determinants of Yield Stress for Semicrystalline Ethylene / Methacrylic Acid Copolymers, ROBERT SCOGNA, RICHARD REGISTER, Princeton University — Reducing the crystal thickness of ethylene/α-olefin copolymers typically results in a decrease in the measured yield stress. However, statistical incorporation of methacrylic acid, also a noncrystallizable comonomer, actually increases the yield stress at room temperature. The yield stress for ethylene/methacrylic acid (E/MAA) copolymers as a function of temperature and test rate is described using a model which accounts for polyethylene crystal plasticity through thermal nucleation of screw dislocations. The effects of temperature and test rate employed in the morphological model are both effective in increasing the yield stress. The model requires a small number of physically reasonable best-fit parameters. Yield stress master curves can be constructed for any material that obeys the model; such curves have been constructed for a low-density polyethylene and five copolymers of varying MAA content from data taken at various strain rates and temperatures. The master curves clearly show that this unusual behavior of the yield stress is caused by the increase in β relaxation temperature with increasing MAA content, as seen via dynamic mechanical testing.

1:51PM B18.00010 On the statistics of Gaussian two and three-dimensional networks: Fluctuations of junctions and collapse driven by structure, MICHAEL LANG, Leibniz-Institute for Polymer Research, Hohe Str. 6, 01069 Dresden, Germany — We investigate ideal Gaussian networks both analytically and with computer simulations using the Bond Fluctuation model with and without excluded volume interactions. The focus of this study is on fluctuations and the collapse of networks with different connectivity and dimensionality. We show that the size of a perfect square 2D network made from $N^2$ Gaussian chains with $N$ monomers each is $R_g \sim N^{3/2} \log(n)$. Thus fluctuations in two-dimensional networks diverge logarithmically with the size of these films while fluctuations of three-dimensional networks $\sim N^{3/2}$ and do not increase with their size. We study the cross-over between two and three-dimensional networks by following the dependence of junction fluctuations on the thickness of films. The results of model systems are compared with more realistic networks in order to understand the effect of disorder on the properties of the network and fluctuations of network junctions.
may be useful for the nano-scale imaging of the soft material. ×

peaks can reveal the contrasts of the interface structure on Ag/Si(111)7 surfaces. It is shown that the spectral intensity of the Gundlach oscillation peaks can vary with observed locations. The spatial mappings of spectral intensities at of samples: bare multilayers of Si/Mo and epitaxial SrTiO3 chemical species and their magnetic properties. We have applied this method, using both rocking curves and sample scans over a wedge profile, to several types by reflection from a multilayer mirror substrate. Combining experiment with x-ray optical simulations can provide information on depth profiles of different

characteristic of Gundlach oscillation can always appear in the tunneling spectrum. We use STS to study Gundlach oscillation on Ag/Si(111)7 × is a phenomenon of field-emission resonance through standing-wave states in the tip-sample gap. No matter if the sample is the thin film or the bulk, peak

oscillations on Ag/Au(111), Ag/Cu(111) and Co/Cu(111) systems, we demonstrate that the work function difference is not the energy shift of the lowest order manifesting in the tunneling spectrum acquired from a metal surface using scanning tunneling spectroscopy. Previous studies relate the energy shift between tuning by gradually approaching the diffusion temperature of the multilayer, which lead to intermixing. We show that core-level spectroscopy directly reflects model system, we demonstrate that this technique is a sensitive tool to characterize the sharpness of a buried interface. We performed controlled interface propulsion nondestructive technique based on atomic core-level shifts to characterize the interface quality of thin film nanomaterials. Our method uses the changes in the electronic structure of the buried interfaces, which ultimately determines the functionality of the nanosized material.

The results showed that the Van der Waals interactions control the bulk modulus below the glass transition. Above the glass transition the internal energy contribution to the bulk modulus is driven by the Van der Waals interaction but a non negligible entropic contribution appeared which at a first order may be considered as independent on the temperature.

Monday, March 10, 2008 11:15AM - 2:15PM — Morial Convention Center 211

11:15AM B19.00001 Spectromicroscopic characterization of Ag surfaces by energy-filtered LEEM Y. FUJIKAWA, T. SAKURAI, Institute for Materials Research, Tohoku University, R.M. TROMP, IBM Research Division, T.J. Watson Research Center — Low energy electrons have been applied successfully for both structural and spectroscopic studies since the early days of modern surface science. While the reciprocal space analysis has been combined with both microscopic and spectroscopic studies, there is still very limited availability of spectromicroscopic analysis because it is not easy to achieve both high spatial and spectroscopic resolution at low energies. We present spectromicroscopic characterization of Ag islands on Si substrates using a newly developed energy-filtered Low Energy Electron / Photo-Electron Emission Microscope capable of 5D (2D spatial + 2D reciprocal + energy) surface analysis. The electron energy loss signal from Ag surface plasmons (SP) was imaged in real space with a resolution of 35 nm or less, while the SP energy dispersion was obtained from a 6 µm diameter area on Ag(111) within ~1 second. Hel photoemission spectra were obtained from a complex Ag island, selecting Ag(111) and Ag(100) areas with a 0.5 µm aperture during PEEM observation. Full dispersion data covering the full reciprocal-energy space were obtained from both surfaces, reflecting their respective symmetries. The ability to perform detailed spectromicroscopic experiments in a standard lab environment is of key importance for nanoscale analysis of novel structures and materials.

11:27AM B19.00002 Enhanced depth-resolution in multilayer nanostructures from standing-wave excited photomission SVEN DOERING, DELTA, TU Dortmund, Germany, MIHAELA GORGOI, RUSLAN OVSYANNIKOV, BESSY, Berlin, Germany, SEE-HUN YANG, IBM Almaden, USA, MARK HJULIBEN, LBNL, Berkeley, USA, FRANZ SCHEAFFER, BESSY, Berlin, Germany, DANIEL BUERGLER, CLAUS SCHNEIDER, Forschungszentrum Juelich, Germany, CHARLES S. FADLEY, LBNL, Berkeley, USA; University of California, Davis, USA; Forschungszentrum Juelich, Germany, WALTER BRAUN, BESSY, Berlin, Germany, CARSTEN WESTPHAL, DELTA, TU Dortmund, Germany — The depth resolution for studying buried layers and interfaces in multilayers with photoemission can be enhanced by exciting with a standing-wave field created by reflection from a multilayer mirror substrate. Combining theoretical analysis of the tunneling differential cross section and experimental measurements of different chemical species and their magnetic properties. We have applied this method, using both rocking curves and sample scans over a wedge profile, to several types of samples: bare multilayers of Si/Mo and epitaxial SrTiO3/La0.7Sr0.3MnO3, and epitaxial MgO on a Fe of top on Au of GaAs/AIAs multilayer. Both soft x-ray excitation at the TU Dortmund DELTA facility and hard x-ray excitation at BESSY II in Berlin have been utilized, with the hard x-rays for the first time permitting the study of deeper layers and interfaces.

11:39AM B19.00003 Interface characterization using atomic core-level shifts, ERIK HOLMSTROM, Universidad Austral de Chile, WEINE OLOVSSON, Kyoto University, IGOR ABRIKOSOV, Linkping University, ANDRES NIKLASSON, Los Alamos National Laboratory, M. F. KOHL, BESSY, Berlin, Germany, OLIVIA KARIS, SVANTE SVENSSON, Uppsala University, SWANTE SVENSSON, Uppsala University, W. BRAUN, BESSY, Berlin, Germany, G. OHRWALL, G. ANDERSSON, B. JOHANSSON, M. MARCELLINI, Uppsala University, W. EBERHARDT, BESSY, Berlin, Germany — We propose a nondestructive technique based on atomic core-level shifts to characterize the interface quality of thin film nanomaterials. Our method uses the inherent sensitivity of the atomic core-level binding energies to their local surroundings in order to probe the layer-resolved binary alloy composition profiles at deeply embedded interfaces. From an analysis based upon high energy x-ray photoemission spectroscopy and density functional theory of a Ni/Cu fcc (100) model system, we demonstrate that this technique is a powerful way to characterize the sharpness of a buried interface. We performed controlled interface tuning by gradually approaching the diffusion temperature of the multilayer, which lead to intermixing. We show that core-level spectroscopy directly reflects the changes in the electronic structure of the buried interfaces, which ultimately determines the functionality of the nanosized material.

1Support from FONDECYT grant: 11070115.

11:51AM B19.00004 Manifestation of Work Function Difference in High Order Gundlach Oscillation, CHUN-LIANG LIN, SHIN-MING LU, WEI-BIN SU, HWA-TE SHIH, BI-FEN WU, YEONG-DER YAO, CHIA-SENG CHANG, TIEN-TZOU TSONG, Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan — Gundlach oscillation (or standing-wave state) is a general phenomenon manifesting in the tunneling spectrum acquired from a metal surface using scanning tunneling spectroscopy. Previous studies relate the energy shift between peaks of the lowest-order Gundlach oscillation observed on the thin film and the metal substrate to the difference in their work functions. By observing Gundlach oscillations on Au(111), Ag/Cu(111) and Co/Cu(111) systems, we demonstrate that the work function difference is not the energy shift of the lowest order but the ones of higher order where a constant energy shift exhibits. Higher order Gundlach oscillations can thus be applied to determine the work function of thin metal films precisely.

1This work is supported by Academia Sinica and National Science Council in Taiwan and has been published in Phys. Rev. Lett. 99, 216103 (2007)

12:03PM B19.00005 Application of Gundlach Oscillation in Scanning Tunneling Spectroscopy on Nano-Scale Imaging, SHIN-MING LU, Academia Sinica Taiwan — Gundlach oscillation observed with scanning tunneling spectroscopy (STS) is a phenomenon of field-emission resonance through standing-wave states in the tip-sample gap. No matter if the sample is the thin film or the bulk, peak characteristic of Gundlach oscillation can always appear in the tunneling spectrum. We use STS to study Gundlach oscillation on Ag/Si(111)/7×7 and Au(111) surfaces. It is shown that the spectral intensity of the Gundlach oscillation peaks can vary with observed locations. The spatial mappings of spectral intensities at peaks can reveal the contrasts of the interface structure on Ag/Si(111)/7×7 and herringbone reconstruction on Au(111) surfaces. The contrast can be attributed to the local variation of the electron transmision which affects the transmission background superposing with Gundlach oscillation in the tunneling spectrum. In our observation, the spatial resolution of the mapping is 1 nm and can be preserved even the tip is away from the sample by 60 angstrom. Gundlach oscillation may be useful for the nano-scale imaging of the soft material.
**12:15PM B19.00006 Standing Friedel waves**

JUN-QIANG LU, CNMS, Oak Ridge National Laboratory, Oak Ridge, TN 37831, X.-G. ZHANG, CNMS & CSMD, Oak Ridge National Laboratory, Oak Ridge, TN 37831, SOKRATEST. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, and MSTD, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — The electron density around defects in a metal is known to exhibit Friedel oscillations. Here, we report simulations that demonstrate a dynamic analogue of the static Friedel oscillation in nanoscale devices. We use a spot gate capacitively coupled to a nanowire or a two-dimensional electron gas, a setup that can be implemented with a sharp STM tip. The application of an AC voltage generates a dynamic standing Friedel wave (SFW), near the spot gate and edges and boundaries. The SFW wave length is controlled by the AC frequency and the device’s Fermi velocity, whereby the latter can be measured. The SFW amplitude exhibits resonant behavior at AC frequencies that are related to eigenenergy spacings in the device, allowing their direct measurement. Spin-polarized SFW may be generated in a graphene nanoribbon.

**12:27PM B19.00007 Molecular Etching of Pure and Mn Intercalated TiSe₂ using an STM**

TIM KIDD, BRETT GAMBL, POLINA SKIRTACHENKO, LAURA STRAUSS, University of Northern Iowa — STM is normally a non-destructive technique. However, some materials, such as the transition metal dichalcogenides (TMDCs), are so weakly bonded that STM measurements performed in air can change the surface topology. We performed STM measurements on single crystals of TiSe₂ and Mn₀.₀₅TiSe₂ in air. Under normal scanning conditions, the surface of both TiSe₂ and Mn₀.₀₅TiSe₂ would spontaneously etch, removing single and double molecular layers. In pure TiSe₂, step edges were unusually rounded and the etching predominately occurred along the scanning direction. In Mn₀.₀₅TiSe₂, the etching occurred even more readily. However, step edges in these samples were much straighter, reflecting the crystal symmetry. The symmetry was also seen in the etching of these samples, as triangular pits were often formed along with the usual etching along the scanning direction. The differences seen in the etching of Mn₀.₀₅TiSe₂ samples indicate intercalated ions can affect both intra- and inter-layer bond strengths. The etched material disappeared completely from the sample, suggesting that TiSe₂ molecules are energized sufficiently to sublime from the sample. This research indicates that the etching process can be controlled to induce complex nanostructures in the surface of TMDCs.

**12:39PM B19.00008 Effect of Surface Stress on the Stiffness of Cantilever Plates**

JOHN SADER, MICHAEL LACHUT, Department of Mathematics and Statistics, University of Melbourne — Measurements over the past 30 years have indicated that surface stress can significantly affect the stiffness of microcantilever plates. Several one-dimensional models based on beam theory have been proposed to explain this phenomenon, but are found to be in violation of Newton’s third law, in spite of their good agreement with measurements. In this talk, we shall review this work and rigorously examine the effect of surface stress on the stiffness of cantilever plates using a full three-dimensional model. This study establishes the relationship between surface stress and cantilever stiffness, and in so doing elucidates its scaling behavior with cantilever dimensions. Use of short nanoscale cantilevers thus presents the most promising avenue for future investigations.

**12:51PM B19.00009 Direct determination of transient heating in a nanoconfined environment by ultrafast electron diffraction**

RYAN A. MURDICK, RAMANI K. RAMAN, YOSHIE MUROOKA, RICHARD J. WORHATCH, CHONG-YU RUAN, Michigan State University — Temperature is generally ill-defined at the statistical limit, as such on the ultrashort time scale and in mesoscopic systems. Understanding the thermal energy relaxation and transport at such limits is key to nanoelectronics and energy research. We report on the development of local temperature determination on the atomic scale using the technique of ultrafast electron diffraction. Lattice heating characteristics are elucidated by determining the dynamical Debye-Waller factor and local bond stretches, allowing the time scale of electron-phonon coupling and local heating at different length scales to be detailed. We compare these measured temperatures with predictions from two-temperature model (2TM) and determine that strongly coupled ‘hot’ phonons dominate lattice heating at short times (10 ps), and cannot explained by 2TMs. Models beyond the 2TM are developed to explain our data. We also discuss other novel heating scenarios at the statistical limits.

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3This research was conducted at the CNMS sponsored at ORNL by the Division of Scientific User Facilities, US DOE.

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1:03PM B19.00010 Surface Femtochemistry with Hyperthermal Energy Ion Beams**

M.P. RAY, R.E. LAKE, C.E. SOSOLIK, Clemson University — We are investigating the interactions of hyperthermal energy ions with ultrathin film Schottky diode devices. Specifically, we apply a bias voltage across the device in order to alter the charge transfer dynamics between an incident ion and the metal surface of the Schottky diode. This is an extension of previous work where thermal energy atoms were used to excite electrons-hole pairs and ballistically transport electrons through an ultrathin metal film [1]. In our experiment, we modify the surface electron energy distribution by ballistically transporting electrons to the surface of the thin film. This allows us to tailor the energy level crossings between the incident ion and the metal film and to change the neutralization probability of the scattered beam. Varying the bias voltage will open the possibility for tunable chemical reactions. Preliminary results are presented and discussed in the context of basic ion-surface interactions. [1] H. Nienhaus, H.S. Bergh, B. Gergen, A. Majumdar, W.H. Weinburg and W. McFarland, Physical Review Letters 82, 446 (1999).

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1We would like to acknowledge support from NSF CAREER CHE-0548111.

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1:15PM B19.00011 Hyperthermal Energy Ion Scattering as a Time Resolved Probe of Pico- to Femtosecond Surface Excitations**

R.E. LAKE, M.P. RAY, C.E. SOSOLIK, Clemson University — Trajectories of hyperthermal energy alkali ions scattered from single crystal metal surfaces are well described by binary classical collisions with a strong dependence on the atom-surface mass ratio. Such simple events allow hyperthermal ion scattering to be used as a time resolved probe for studying novel surface effects such as femtosecond scale electron transport and ballistic electron excitations. In this talk, three ion scattering cases from the 1-1000 eV energy regime are discussed. K⁺ scattered from Ag(100) is compared to Na⁺ scattered from Cu(100) in terms of interaction potential, image charge effects and neutralization probability. Secondly the heavy atom Cs⁺-Ag(100) system will be presented including a discussion of an anomalous high energy peak possibly attributable to a collective surface response. Finally a method for probing hot electron excitations by an alkali beam scattered from a biased atomically ordered ultrathin film device will be discussed including charge transfer predictions based on rate equations and quantum mechanical I/N and dynamic matrix renormalization group codes.

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1We would like to acknowledge support from NSF-CHE-0548111.

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1:27PM B19.00012 An Investigation of Nitride Formation on InP Surface After Nitrogen Ion implantation**

MOHAMMAD REZA HANTEHZADEH, Azad University — The effect of nitrogen ion implantation and change in physical characteristics of InP [100] surface after nitrogen ion implantation is investigated. The energetic 30 keV nitrogen ions with different doses were implanted into [100] InP surface at about 500-700 k. The formation of different phases of indium nitride and change in surface morphology after the implantation is studied. The annealing effect on change in nitride phase in a nitrogen environment at temperatures above 900 k is observed. The morphology and phases of the surface after ion implantation is characterized using AFM and XRD.
1:39PM B19.00013 Sputter Deposition System for High Throughput Fabrication of Composition Spread Thin Films

JOHN GREGOIRE, FRANK DISALVO, HECTOR ABRUNA, ROBERT BRUCE VAN DOVER, Cornell University — We describe a custom built sputtering system that can deposit composition spreads in an effectively UVH environment but which does not require the high-throughput paradigm to be compromised by a long pumpdown each time a target is changed. The system employs four magnetron sputter guns in a cryoshroud (getter sputtering) which allows elements such as Ti and Zr to be deposited with minimal contamination by oxygen or other reactive background gases. Other features of the deposition system will be presented, most notably the ability to quickly measure deposition profiles from individual deposition sources. We discuss the possibility of calculating codeposited film composition from these profiles, noting that codeposition affords resputtering phenomena which are absent in single-source deposition. To demonstrate the efficacy of this system, we describe our study of combinatorial libraries of electrocatalyst materials for fuel cell applications. This study includes a high-throughput parallel screening of composition spreads using a fluorescence indicator.

1Supported by the National Science Foundation Grant No. PHY-0646718.

1:51PM B19.00014 Discharging Optics in Vacuum

MARK GIRARD, DENNIS UGOLINI, Trinity University — We have studied using UV illumination to remove excess surface charge from fused silica optics. We commissioned and calibrated a commercial Kelvin probe to measure the surface potential of charged optics in vacuum. Using a Xenon light source and a monochromator, we directed UV light at the sample and were able to remove the excess charge. We determined that the discharging rate scaled linearly with the intensity of the light and the charge density on the surface. By varying the wavelength of the light, we saw a peak discharge rate at 215nm in both uncoated and coated optics. The Kelvin probe also allows us to study the sign of the charge carriers and other techniques for charge removal.

2:03PM B19.00015 Ordering process in metallic thin films investigated with angle-resolved photoelectron spectroscopy

DAH-AN LUH, National Central University, CHENG-MAW CHENG, National Synchrotron Radiation Research Center, CHI-TING TSAI, National Central University, KU-DING TSUEI, National Synchrotron Radiation Research Center, JIAN-MING TANG, University of New Hampshire — We report the observation of the ordering process in real time of a Ag thin film on a Au(111) surface by measuring the in-plane dispersion of quantum well states using temperature-dependent angle-resolved photoelectron spectroscopy. Low-temperature deposited Ag films on a Au(111) substrate were annealed to yield atomically flat films, and the in-plane dispersion of quantum well states was measured in real time during annealing. Our results revealed that isolated ordered patches, fully crystallized along the surface normal, are formed as an intermediate step in the process of film crystallization. We observed the transition from localized states in a partially ordered film to free-electron-like states in a fully ordered film. This process may be general in many other systems of metal thin films.

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11:15AM B20.00001 Growth instabilities and adsorbed impurities: Nanostructuring of vicinal surfaces controlled by adsorbates

AJMI BHADJ HAMOUDA, T.L. EINSTEIN, U. of Maryland, College Park, P.E. HOGGAN, A. PIMPINELLI, LASMEA, U. Blaise-Pascal, Clermont-2 — A kinetic Monte Carlo study of the meandering instability of a vicinal surface growing by step flow is performed. Impurities are co-deposited during growth, and they are shown to be responsible for quantitative and qualitative modifications of the surface morphology. In particular, impurities make adatom diffusion less dependent on the deposition rate, affecting thus the wavelength of the meandering. Impurities also act as nucleation centres, causing small stepped pyramids to appear on the surface. Comparison with step-flow experiments on vicinal Cu(100) make plausible the hypothesis that many previously unexplained features of the meandering instability in this system are due to impurities. The density of nano-pyramids can be tuned by varying the impurity concentration. Our results show also that the step bunching instability is strongly affected by adsorbed impurities having lower diffusion rate than adatoms. Such impurities slow the adatoms diffusion and weakens the instability, even removing it at large impurities concentration.

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

11:27AM B20.00002 Effects of deposition angle in metal(100) epitaxial growth

JACQUES G. AMAR, VALERY BOROVIKOV, YUNCIS SHIM, University of Toledo — The effects of oblique incidence on the surface roughness and morphology in Cu/Cu(100) epitaxial growth are investigated via multiscale kinetic Monte Carlo simulations in which the effects of shadowing and short-range (SR) and long-range (LR) attraction during deposition are taken into account via molecular dynamics simulations. Somewhat surprisingly, while the effects of deposition angle are found to depend strongly on deposition angle even for moderate deposition angles. These results resolve a long-standing puzzle regarding the growth behavior of Cu/Cu(100) over this temperature range. We also find that while the effects of shadowing and SR attraction play important roles, for moderate deposition angle the effects of LR attraction are relatively weak. Our results also demonstrate that, in general, the effects of deposition angle must be considered in low-temperature growth even for moderate deposition angles. Results for the surface morphology and roughness at higher temperatures and for very large deposition angles are also presented and compared with experiments.

11:39AM B20.00003 Shape fluctuations of small Pb(111) islands at low temperatures

M. HUPALO, M.C. TRINGIDES, Iowa State University and Ames Laboratory of US-DOE — With STM we have measured shape fluctuations of monolayer Pb(111) islands grown on top of Pb mesas of controllable height to determine their step energy. Islands as small as 10nm in diameter were used to test the limit of the thermodynamic analysis. It found that the mean square deviations of the fluctuations obey a linear relation on RT where R is the island radius and T the temperature in agreement with the standard analysis. The extracted step energy 140eV/atom is in good agreement with the one obtained in the literature on islands of much larger sizes. Fluctuation magnitude of bilayer island grown on top of 5-layer island (which corresponds to a magic 7-layer height) are much lower and the corresponding step free energy is three times higher than for monatomic steps.

1Ames Lab is supported by Department of Energy-Basic Sciences under Contract DE-AC02-07CH11358.
11:51AM B20.00004 Connector Model for Many-Body Interactions at Surfaces from First Principles, YOGESH TWIARY, KRISTEN FICHTHORN, The Pennsylvania State University — First-principles calculations based on DFT indicate that pair, trio, four- and five-body atomic interactions are significant in Al clusters on Al(110). These many-body interactions are a signature of “elastic screening” of long-ranged, substrate-mediated, elastic interactions between atoms in dilute adlayers by direct bonding and short-ranged substrate relaxation in dense clusters. As a consequence of this screening, we developed the Connector Model to effectively describe the energies of compact clusters. Adsorbate structures and interactions are described in terms of single-atom, many-body connector units, which link to one another to form the structures that can occur in thin-film and crystal growth. The additive connector energies can be effectively incorporated into a lattice-based Hamiltonian to study thermodynamics and kinetics at surfaces. The Connector Model is considerably more efficient than lattice-gas Hamiltonian approaches, which would require a large number of terms to accurately capture many-body effects. Details of the connector model and its application to predicting the shapes of compact clusters on Al(110) including the chain-to-island transition will be discussed. This model can be extended to other crystalline surfaces.

1NSF DMR 0514336

12:03PM B20.00005 Double-layer island decay on Ag(111): A molecular dynamic simulation, BERK ONAT, Informatics Institute, Istanbul Technical University, Maslak, 34469, Istanbul, Turkey, SONDAN DURUKANOGLU, Department of Physics, Istanbul Technical University, Maslak, 34469, Istanbul, Turkey — We have performed molecular dynamic simulations to investigate double-layer island decays on Ag(111) using the interaction potentials based on the embedded atom method with a specific aim to observe the effect of varying island size and temperature on interlayer mass transport between two layers of the adatom islands. Our preliminary results indicate that decay rates of adatom islands show different characteristics with varying adatom island size. From an analysis of MD simulations, we further examine how the activation barriers for several diffusion processes taking place during adatom island decay change with respect to varying temperature and island size.

This work was partially supported by TUBITAK under Grant No. TBAG-105E067 and TBAG-106T567. B. Onat acknowledges the graduate student fellowships by Advanced Technologies program of Turkish State Planning Organization.

Current address: Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

12:15PM B20.00006 Kinetics of Facile Bilayer Island Formation for Ag on NiAl(110), J.W. EVANS, YONG HAN, D.-J. LIU, BARIS UNAL, F. QIN, D. JIN, C.J. JENKS, P.A. THIEL, Iowa State University — STM studies reveal that deposition of Ag on NiAl(110) at 27 K and above leads to bilayer-by-bilayer growth of a nearly-strain-free film with Ag(110) structure [1]. This growth mode is attributed to Quantum Size Effects (QSE) associated with electron confinement in the Ag film. Our focus here is on analysis the initial nucleation and growth of bilayer Ag(n) islands on NiAl(110) which is facile even at 127K despite requiring uphill transport of Ag. DFT analysis for supported Ag films determines adatom adsorption energies (which display QSE), interaction energies, and various relevant diffusion barriers. Kinetic Monte Carlo simulation of an atomistic lattice-gas model incorporating these energies highlights the role of strongly anisotropic interactions in facilitating bilayer island formation.


12:27PM B20.00007 Self-organization and pattern selection under nanosecond pulsed laser-induced melting of ultrathin metal films, RAMKI KALYANARAMAN, CHRISTOPHER FAVAZZA, JUSTIN TRICE, Dept. of Physics, Washington University in St. Louis, RADHAKRISHNA SURESHKUMAR, Energy, Environmental and Chemical Engineering, Washington University in St. Louis — When an ultrathin metal film is rapidly melted by nanosecond (ns) laser pulses, ensuing hydrodynamic instabilities and/or fluid flow due to surface tension gradients lead to self-organizing patterns of ordered nanostructures. The extremely fast heating O(100 K/ns) and resolidification (O(10 K/ns) in such ns melting experiments permits quenching in of the morphology. Thus, multiple pulses of such fast melting/resolidification cycles in the film allow different stages of the patterning process to be identified and studied. We show that pattern formation via a thin film hydrodynamic dewetting instability and thermocapillary flow can compete and the dominating mechanism is one which has shorter time scale. We have explored this behavior for a large variety of metals, including Ti, V, Mn, Fe, Co, Ni, Cu, and Ag. This ns melting approach permits the robust self-organization of a wide variety of nanoscale structures, including nanoholes, nanostars, nanoparticles and nanowires.

R.K. and R.S. acknowledge support by the NSF through CAREER Grant No. DMI-0449258 and No. CTS-0335348, respectively.

12:39PM B20.00008 Quantum engineering of apparent tunneling height in ultra thin Pb films, JUNGDAE KIM, SHENGYONG QIN, CHIH-KANG KEN SHIH, Department of Physics, University of Texas at Austin — The thickness dependence of tunneling decay constant (κ) for ultra thin Pb films is studied with various sample biases by using low temperature STM. It is found that quantum well states (QWS) have a strong influence on the tunneling decay constant κ. While the decay constant versus layer thickness (κ vs. L) clearly shows bilayer oscillations, we found that the apparent contrast in κ vs. L also show strong bias dependence. Depending on the bias voltage, contrast reversal in the apparent oscillation of κ vs. L can be precisely tuned when the tunneling into the sample empty states. This result also shows that κ-oscillation does not necessarily imply the work function oscillation. We further show that in this case, the parallel component of crystal momentum plays a critical role in tunneling process and is largely responsible for the observed phenomena. On the other hand, at negative sample bias, we show that the measured decay constants well reflect the variation of surface work function. In this case, the layer-dependent surface work functions indeed show bi-layer oscillations and the signature of phase slip due to non-perfect phase matching between Fermi wavelength and the vertical lattice constant.

1NSF-IGERT DGE-0549417; NSF-FRG 26-1126-8750

12:51PM B20.00009 Why Is The Size Dependence Of the Scanning Tunneling Microscopy Workfunction Order Of Magnitude Larger Than That Of Photoemission?, WEI-XUE LI, XIN LIU, Dalian Institute Of Chemical Physics, CAS, Dalian, China, S.B. ZHANG, National Renewable Energy Laboratory, Golden, CO, U.S.A. — Quantum size effect (QSE) has been studied extensively, as a primary driving force for nano technology. Recent scanning tunneling microscopy workfunction of ultrathin Pb(111) film found however order of magnitude larger of QSE than that of photoemission. By first-principles calculations, we show that the QSE is not merely a size effect but symmetry driven: being maximal at the Σ point (i.e., the center of the surface Brillouin zone) derived from interlayer coupling of p_x orbital, but could be vanishingly small at other symmetry points from in-plane p_{x,y} orbital. The Σ valley states have the slowest decay. Thus they are the ones being picked up by near-field techniques such as the scanning tunneling spectroscopy. While whole surface Brillouin zone contributes equally to photoemission, and only marginal QSE effect occurs. For this reason, symmetry could be essential for all near-field physics and chemistry.
1:03PM B20.00010 Tuning Surface Energy Landscapes in Metallic Quantum Films using Alkali Adsorbates 1. ALEXANDER KHAJE TO RIAN, SHENGYO QIN, Dept Physics; U. Texas Austin, WENGUANG ZHU, U. Tennesse-Knoxville; Oak Ridge National Laboratory, HOLGER EISELE, TU-Berlin, ZHENYU ZHANG, U. Tennesse-Knoxville; Oak Ridge National Laboratory, CHIH-KANG SHIH, Dept Physics; U. Texas Austin — Quantum confinement shows a strong interplay with growth and kinetics in thin metal systems where the Fermi wavelength has a special relationship to the surface normal lattice constant. In the case of Pb/Si(111) systems, this relationship reveals an interesting thickness-dependent bilayer oscillation in the density of states and surface energy up to a phase. In this paper, we report on a novel effect: tuning of the energy landscape of a flat-top quantum Pb mesa using Cs adsorbates. Using STM/STS, we show that depositing Cs adsorbates on a thin Pb mesa promotes quantum stable Pb islands on preferentially unstable thicknesses. Thickness-dependent nanoisland densities show a strong bilayer oscillation correlating with quantum stability. By modifying the Cs coverage on the mesa surface, we can tune the lateral size distribution of the nanoislands and the overall amplitude of the island density oscillation. Nanoisland formation is linked to a step decoration of Cs adatoms along the step edge of the nanoisland.

1 NSF-IGERT DGE-0549417; NSF-FRG 26-1126-8750

1:15PM B20.00011 Super-oscillations in the Interlayer Lattice Relaxation of Quantum Pb Films. 1. YU JIA, Zhengzhou University, China, BIAO WU, Institute of Physics, CAS, China, T.L. EINSTEIN, University of Maryland, H.H. WEITERING, The University of Tennessee & ORNL, ZHENYU ZHANG, ORNL & The University of Tennessee — Using first-principles total energy calculations, we study the interlayer relaxation in lead films and observe oscillations of the interlayer lattice relaxation with layer number (distance from vacuum) and with film thickness. By analyzing the charge distribution along the direction perpendicular to the film, we show that the former oscillations of lattice relaxation are induced by Friedel interlayer relaxation in lead films and observe oscillations of the interlayer lattice relaxation with layer number (distance from vacuum) and with film thickness.

1:27PM B20.00012 Modifying the Adsorption of Molecules at Metal Surfaces by Quantum Confinement of Electrons, LEVAN TSKIPURI, ROBERT BARTYNSKI, Rutgers University — We have studied the bonding of CO on several ultrathin Cu and Co films that exhibit metallic quantum well (MQW) states, whose energies change as a function of overlayer thickness, using inverse photoemission (IPE), reflection-absorption infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD). For Co system, which has unoccupied MQW states that do not cross the Fermi level, a CO 2r-induced feature is observed in IPE at 3.8 eV above E_F. CO desorbs at 375 K (30 K lower than for hcp Co surfaces) and a second TPD feature at 230 K appears upon low temperature (∼100K) dosing. These TPD peak temperatures change as a function of film thickness and are correlated with two different C-O stretch vibrational frequencies observed in the IR spectra. The intensity of the C-O stretch feature in IRAS spectra, and the peak CO desorption temperature in TPD from CO on Cu MQWs both show modulations that are correlated with MQW states crossing the EF. We have also studied the influence of MQW states on the adsorption properties of the dimethyl disulfide (thiol) molecule (CH_3S_2), which forms a self-assembled monolayer when adsorbed on the Cu(100) surface.

1:39PM B20.00013 Crystal structure and height selection for Indium growth on Si(111) interfaces 1. J. CHEN, M. HUPALO, M. JI, C.Z. WANG, K.M. HO, M.C. TRINGIDES, Iowa State University and Ames Laboratory of US-DOE — The growth of In/Si(111) has been studied with SPA-LEED and STM to identify whether QSE-driven height selection with mono-disperse distribution is possible. The motivation is to discover other metals besides Pb/Si(111) with high degree of self-organization. Indium growth only on one substrate (Si(111)- Pb-α < 3x√3/3) has resulted in uniform height In(111) 4-layer flat top islands (with the fcc(111) orientation different from the bct In bulk structure). This allotropic transition is observed at low temperatures T<250K and coverages θ<0.1ML. Otherwise bct(110) oriented In islands are observed with continuously increasing height/size aspect ratios. These results suggest two stabilizing energetic effects for the fcc In(111) height selection i.e. Quantum Size Effects (QSE) stabilize uniform height and orientation dependent surface energy favours the different crystallography. The contribution of each effect was studied with first principles calculations and both the height selection and the allotropic transition can be quantitatively explained. -/a

1 Ames Lab is supported by Department of Energy-Basic Sciences under Contract DE-AC02-07CH11358

1:51PM B20.00014 Non-classical scaling in the Pb/Si(111) coarsening at low temperature 1. MYRON HUPALO, Iowa State University Ames Lab-USDOE, R. FENG, E.H. CONRAD, C.A. JEFFREY, P. F. MICIELI, S. HAYDEN, M. GRAMLICH, P. J. RYAN, C. KIM, MUCAT, Advanced Photon Source, Argonne National Laboratory, M.C. TRINGIDES, Iowa State University Ames Lab-USDOE — Recent coarsening experiments monitoring the evolution of a mixture of stable and unstable islands in Pb/Si(111) towards a mono-disperse T-layer height distribution have revealed novel features that extend the classical curvature driven growth. Two complementary techniques are used, X-ray scattering and STM. In particular the coverage θ, temperature T and flux F dependence are the opposite of what is expected from the classical analysis. The coarsening time τ increases with increasing temperature T, coverage θ and decreases with increasing flux rate F according to the scaling relation τ F^c. These paradoxical results can be understood from the island stability dependence on lateral size L in addition to the QSE-driven well-analyzed height dependence. The decay constant of an unstable island is an increasing function of its lateral size and for sizes larger than L≃50nm the unstable states do not decay but grow in the next stable height. Since the lateral size increases with T, θ and decreases with F this can account for the novel coarsening results.

1 Acknowledgement: NSF(DMR0706278), PRF(41792-AC10), Advanced Photon Source(DOE), Ames Lab is supported by Department of Energy-Basic Sciences under Contract DE-AC02-07CH11358

2:03PM B20.00015 Surface, quantum well, and bulk states in Ag films, NATHAN SPEER, UIUC, CHING WEI, Academia Sinica, TOM MILLER, TAI CHIANG, UIUC — Atomically uniform Ag films grown on Si(111) substrates show, in addition to the usual Shockley Surface state, multiple surface states in pockets within the d-band manifold as observed by angle-resolved photoemission spectroscopy. At low coverages, quantum well states are resolved. As the film thickness increases, quantum well states evolve into the bulk band continuum plus separate surface states. The results are compared to a density functional theory calculation.

Monday, March 10, 2008 11:15AM - 2:03PM –
Session B21 DCP: Focus Session: Clusters, Cluster Assemblies, Nanoscale Materials I
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We have also shown that all transition metals including the f-block elements can be doped inside Sn cages, confirming their structural robustness, as well as demonstrating chemical tuning of their electronic, magnetic, and catalytic properties.

$n = 16-18$ possess unprecedented hollow cage structures. We have been able to successfully dope a variety of transition-metal atoms into the empty spaces.

-PES with theoretical calculations has become an effective approach to obtain structural information for small and medium-sized clusters. We present a synergistic effort combining PES with theoretical calculations to examine the geometries, stability, vibrational frequencies and optical properties of Si clusters. It is proposed that the oxygen enrichment needed to form silicates in interstellar space, starting from SiO molecules can occur via two processes: (1) Chemically driven compositional separation in [SiO] motifs resulting in oxygen rich and oxygen poor regions, and (2) reaction between SiO$_m$ clusters leading to oxygen richer and poorer fragments. Theoretically calculated optical and infrared spectra of SiO$_m$ clusters exhibit features observed in the extended red emissions and blue luminescence from interstellar medium indicating that the SiO$_m$ fragments could be contributing to these spectra.

Supported by the National Science Foundation.

Recent ab initio studies have predicted large electric dipole moments in neutral Na clusters. We performed an electric deflection experiment on these clusters at 20 K and have found upper bounds on their dipole moments that are orders of magnitude smaller than predicted, and consistent with zero.

Supported by the National Science Foundation.

Theoretical studies on the geometry, electronic structure and spin multiplicity of Sc, Ti and V doped Na$_n$ clusters have been carried out within a gradient corrected density functional approach. Two complementary approaches including all-electron calculations on free clusters, and supercell calculations using planewave pseudopotential and projector augmented wave formalisms have been carried out. It is shown that spin magnetic moments of the transition metal atoms, the magnitude of host polarization, and the sign of the host polarization all change with the number of alkali atoms. In particular the transition metal atoms are shown to attain spin moments that are higher than their atomic values. The role of hybridization between the transition atom d-states and the alkali sp-states is highlighted to account for the evolutions in the spin moments and host polarization.

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Supported by the National Science Foundation.

We gratefully acknowledge support from the Department of Energy (DE-FG02-02ER46009)
Cooperative effect between electronic and geometric structures in binary clusters of superatoms, ATSUHIKO NAKAJIMA, Keio University & JST-CREST — The fabrication of cluster-assembled materials is dependent upon finding a suitable building block for a cluster that is chemically stable and that interacts weakly with other clusters of the same material. For designing the characteristics of clusters, binary systems are very important to create functionality of materials, and application of hetero-atom encapsulated clusters were examined experimentally. For aluminum-based binary superatoms of Al12X, both experimental and theoretical results show that Al12Si has high ionization energy and low electron affinity, and Al12P has low ionization energy, both with the icosahedral structure having a central Si or P atom, revealing that Al12Si and Al12P exhibit rare-gas-like and alkalai superatoms, respectively. Experiments confirmed the possibility that the change in the total number of valence electrons on substraction could produce ionically bound binary superatom complexes; the binary cluster salts (Al12P)· F− and (Al12B)· CS−. For silicon-based binary superatoms of MnOSi6, on the other hand, results obtained by mass spectrometry, anion photoelectron spectroscopy, and adsorption reactivity towards H2O show that the neutral cluster doped with a group-4 atom exhibits a nuclear and an electronic geometric closing at n=6. The MnSi6 cluster with a group-4 atom undergoes an electronic change in (i) the number of valence electrons when the metal atom is substituted by the neighboring metals with a group-3 or -5 atom, and in (ii) atomic radii with the substitution of the same group element of Zr and Hf. The reactivity of a halogen atom with the MnSi6 clusters reveals that VSi12F forms a superatom complex with ionic bonding.

Stability and Magnetic Coupling between Mn doped Stannaspherenes, ANIL KANDALAM, GANG CHEN, PURU JENA, Virginia Commonwealth University — The discovery of carbon fullerenes has stimulated considerable interest in the search of cage clusters involving not only group IV elements but also metallic systems. The recent discovery of stannasphene, a highly stable Sn12 0 hollow cage cluster with a reported diameter of 6.1 Å has triggered a renewed interest in the search for stable endohedral cage complexes with 3d transition metal atomic dopants. It is anticipated that these complexes may carry large magnetic moments and can be used as building blocks for novel magnetic materials. We report the first density functional theory based study of the interaction between two Mn doped stannaspherenes (Mn@Sn12) and show that Mn@Sn12 is not only highly stable and carry a magnetic moment of 5µB, but the clusters retain their structural identity even when they interact with each other. Equally important, the magnetic coupling depends strongly on the orientation of the clusters. We believe that these new results would encourage the scientific community to explore the possibility of synthesizing novel magnetic materials with magnetic element doped Sn12 clusters as building blocks.

11:15AM B22.00001 In-crystal carriers in organic single crystal transistors, JUN TAKEYA, Y. TOMINARI, M. YAMAGISHI, Y. IWASAKI, Osaka University, OSAKA UNIVERSITY TEAM — The intrinsic semiconductor character of organic semiconductors, consisting of one molecular species, causes peculiar features different from those of doped inorganic semiconductors, when they are built in field-effect transistors (FETs). The effect can be most drastic with purified organic single crystal devices because of their minimized impurity (defect) concentrations of ~ 10^14 cm^-3, resulting in relatively long length scale (more than 1 µm) of band bending and carrier distribution in the direction of the crystalline thickness. In this presentation, we report effects of the in-crystal carriers in two FET structures of clean rubrene single-crystals with the thickness comparable to the length scale of the distribution. With a double-gate device incorporating two transistor structures on the both sides of the crystal, we found that each transistor cross-talks with each other, inducing high-mobility (higher than 30 cm^2/Vs) carriers inside the crystal. The similar cross-talking events are observed also for a device with an acceptor layer of F3-TCNQ on one side of the rubrene crystal.

11:27AM B22.00002 Defect healing at room temperature in pentacene thin films and improved transistor performance, WOLFGANG KALB, FABIAN MEIER, KURT MATTENBERGER, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We observed a healing of defects at room temperature in the prototypical organic semiconductor pentacene. Pentacene thin-film transistors were fabricated and characterized by in situ gated four-terminal measurements. Under high vacuum conditions (base pressure of order 10^-10 mbar), the device performance is found to improve with time. The effective field-effect mobility increases by as much as a factor of two and the contact resistance decreases by more than an order of magnitude. Oxygen/nitrogen exposure and annealing experiments show the improvement of the electronic parameters to be due to a reduction in the density of shallow traps, while the energetic deeper traps are essentially unaffected. This peculiar effect is a direct consequence of the weak intermolecular interaction which is characteristic of organic semiconductors.

11:39AM B22.00003 Impurities and carrier trap formation in rubrene, LEONIDAS TSETSERIS, Aristotle University of Thessaloniki, Greece, and Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Rubrene has emerged recently as a very promising system for applications in organic electronics. In particular, measured carrier mobilities of rubrene films have been among the highest values reported for organic semiconductors. Here we present the results of first-principles calculations on impurities in rubrene crystals. We find that the most stable atomic H defect induces deep traps in the energy band gap of this prototype organic semiconductor, but we further show that the formation of a stable pair of vicinal H impurities eliminates these traps. We thus establish a dual role of hydrogen in carrier trap formation in rubrene devices. We also find that the incorporation of oxygen and water-related impurities is energetically favorable, and we address their possible role in the appearance of energy levels in the band gap of rubrene. Finally, we discuss the relevance of our findings for the development and operation of rubrene-based devices. This work was supported in part by DOE Grant DEFG0203ER46096.
11:51AM B22.00004 Organic Field Effect Transistors Based on Micro and Nano-sized Single Crystalline Semiconductors. ZHENAN BAO — Organic single crystals are of interest for fundamental charge transport studies. Recently, we have shown that organic semiconductor single crystals can be patterned over a large area using vapor phase growth method. This opens up new possibilities of using organic single crystals for high performance devices. In this talk, I will present our recent work in solution deposition of single crystals by various methods and their device performance.

12:27PM B22.00005 Field-effect modulated Seebeck coefficient in pentacene and rubrene. K.P. PERNSTICH, B. ROESSNER, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland — We report on the first study of the charge carrier concentration and the temperature dependence of the Seebeck coefficient $S$ for two prototypical organic semiconductors measured in a field-effect transistor (FET) structure. As a basic transport property of solids, the Seebeck coefficient provides deep insights into the nature and dynamics of charge carriers. Using a FET structure enables the variation of the Fermi-level position in the active semiconductor region while measuring $S$, which is essential for determining individual contributions to the thermopower. The sign of the measured Seebeck coefficient is consistent with hole transport, and $S$ is in the range of 0.3-1 mV/K, it is independent of temperature between 295 K and 200 K, and interestingly it decreases for both semiconductors as $S \propto |V_a|$. The measured $S$ is quantitatively described by $S = (k/e)(E(V_a)/kT + A)$. The Fermi-level position $E(V_a)$ is obtained from analyzing the transistor's characteristic which then allows to calculate the parameter $A$. For both semiconductors we find that $A$ is in the range of 1.7-3.6, just as in conventional semiconductors. The results are well described by solely considering a realistic density of in-gap trap states and band-like transport of quasiparticles that are subjected to scattering. There is no need to invoke self-trapping of massive charge carriers.

12:39PM B22.00006 Contact-correlated bias stress instability in pentacene thin film transistors. K. TSUKAGOSHI, S.D. WANG, T. MINARI, T. MIYADERA, Y. AYOAGI, RIKEN, Saitama 351-0198 and CREST-JST, Saitama 332-0012. Japan — The bias stress effect and large contact resistance are the remaining problems for practical applications of organic thin film transistors (OTFTs). The bias stress effect in top-contact pentacene TFTs was observed to be correlated with the metal/organic contact. The drain current decay under the bias stress condition results from the combination of the contact resistance change and the channel resistance change arising from the threshold voltage shift in the channel. The transistors with the different contacts (gold and copper) show the very similar channel properties. On the other hand, the bias-stress-induced contact resistance change in the gold transistor is much larger than the corresponding channel resistance change, so that the bias stress effect can be even dominated by the gold contact. In contrast, the copper contact is more stable, showing the small contact resistance change. The temperature variance measurements on contact resistance indicate that, the gold contact has a wider trap distribution compared with the copper contact, that is, there are much more deep trap states at the gold contact. Therefore, the time-dependent charge trapping in the deep traps is proposed to be the mechanism of the bias stress effect in OTFTs.

12:51PM B22.00007 Negative Magnetoresistnace of Organic Field Effect Transistors. MASAYA NISHIOKA, YEONBAAE LEE, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota, YU XIA, DANIEL FRISBIE, Department of Chemical Engineering and Materials Science, University of Minnesota — The magnetoresistance (MR) of organic field effect transistors has been studied. Both pentacene films and tetracene single crystal and rubrene single crystal devices exhibit negative MRs of up to 1.2 % at 9 T. This has been demonstrated to not be contact related. The effect has been found to increase with decreasing temperature between 150 and 300 K. On the other hand, this effect is not strongly affected by the magnetic field direction. The phenomenon may result from the action of the magnetic field on the hopping transport of carriers. However, the possibility of a magnetocapacitance effect that would increase the number of carriers cannot be ruled out.

1:03PM B22.00008 Pentacene Thin-Film Transistors With Organophosphonate Self-Assembled Monolayer Modified Gate Dielectrics. IAN HILL, MATTHEW MCDOWELL, Dalhousie University, JOSEPH MCDERMOTT, JEFFREY SCHWARTZ, STEVEN BERNASEK, JAEHYUNG HWANG, ANTOINE KAHN, Princeton University — Organophosphonate-based self-assembled monolayers synthesized from aliphatic, aromatic, and heterocyclic moieties were used to modify silicon dioxide gate dielectric in pentacene organic thin-film transistors. Striking improvements in the subthreshold performance of these devices is noted, with a dependence on the molecular species used in fabricating the monolayer. All modified gate dielectrics outperform the untreated surface. As determined by parameters such as the subthreshold slope, threshold voltage magnitude and uniformity, and the on/off ratio, the aromatic species outperform the heterocyclic species, which outperform the aliphatic species. Origins of the improvement, based on energetic alignment of the molecular levels of the SAM and the pentacene, and charge trap densities will be discussed.

1:15PM B22.00009 Percolative Effects on Noise in Pentacene Transistors. BRAD CONRAD, WILLIAM CULLEN, WINSTON YAN, ELLEN WILLIAMS, University of Maryland - College Park — Noise in pentacene thin film transistors has been measured as a function of device thickness from well above the effective conduction channel thickness to only two conducting layers. Over the entire thickness range, the spectral noise level is 1/f, and the noise parameter varies inversely with gate voltage, confirming that the noise is due to mobility fluctuations, even in the thinnest films. Hooge's parameter varies as an inverse power-law with conductivity for all film thicknesses. The magnitude and transport characteristics of the spectral noise are well explained in terms of percolative effects arising from the grain boundary structure. http://arxiv.org/abs/0710.2700v2

1:27PM B22.00010 Surface-Treatment Effects on the Pentacene-Based Organic Field-Effect Transistors with Anodized Gate Dielectrics. YEON TAEK JEONG, CHRISTOPHER LOMBARDO, DAVIANNE DUARTE, ANANTH DODABALAPUR, The University of Texas at Austin — The realization of low operating voltage organic field-effect transistors (OFETs) is technologically important with many methods having been proposed to achieve this goal. The use of anodized high-k dielectrics is very promising in that the approach is applicable to obtaining gate dielectrics at low temperature. We report on the device characteristics and proper surface-treatment effects on low voltage OFETs with anodized Ta2O5 and SiO2 gate dielectrics. Pentacene-based OFETs with anodized Ta2O5 gate dielectric obtained from an e-beam-evaporated and a sputtered Ta thin film exhibited the saturation mobility of 0.52 cm2/Vs and 0.45 cm2/Vs at Vds = -10V, respectively. Moreover, a hexamethyldisilazane (HMDS) and a mono-dodecyl phosphate surface treatment resulted in enhanced mobility and significantly reduced gate leakage current. In the case of anodized SiO2 devices, an octadecyltrichlorosilane (OTS) treatment increased the saturation mobility from 0.38 cm2/Vs to 0.88 cm2/Vs at Vds = -10V. The OTS treatment also proved to reduce gate leakage current by more than 90%. In related work, we will discuss the fabrication of all-organic dual-channel devices. These devices are promising because of their probable applications to organic sensing and CMOS transmission gates.

3 Work supported by the National Science Foundation through the University of Minnesota Materials Research Science and Engineering Center under Grant No. NSF/DMR-0212032.

2This work was supported by NIST under contract #70NANB6H6138, by the LPS, and by the UMD NSF-MRSEC under grant DMR 05-20471. We are grateful to M. Ishigami and D. Dougherty for setting up the noise measurements and for extremely insightful discussions.

3This work was supported by NIST under contract #70NANB6H6138, by the LPS, and by the UMD NSF-MRSEC under grant DMR 05-20471. We are grateful to M. Ishigami and D. Dougherty for setting up the noise measurements and for extremely insightful discussions.
1:39PM B22.00011 Drift mobility and frequency response of diode connected organic field effect transistors, BRIAN COBB, ANANTH DODABALAPUR, University of Texas at Austin — Common methods of estimating the mobility of carriers in organic field effect transistors (OFETs) include extraction from output or transfer characteristics. Mobilities extracted from transfer curves are realistic only in certain steady-state regimes. Optical time-of-flight methods measure charge mobility in directions perpendicular to the semiconductor-dielectric interface, perpendicular to the direction of transport in a functioning OFET. We have developed a method that allows the extraction of the drift mobility of charges through an active channel in an OFET by measuring the frequency response of a diode connected device. An AC signal of varying frequency was applied to both the Gate and Drain nodes, while the rectified output voltage was measured at the Source node using an oscilloscope. This rectified voltage remains relatively steady at lower frequencies, then displays a marked fall. This pole was found to correspond to the transit time of the carriers through the channel. The fabrication of the OFETs, calculation of drift mobility from the frequency of the pole, and the effects of varying channel length will be reported.

1:51PM B22.00012 Field-induced polymorphous disorder and bias-stress instability of pentacene organic thin-film transistors, MASAHIKO ANDO, Hitachi Cambridge Laboratory, CLAUDIA DUFFY, JESSICA WINFIELD, Cavendish Laboratory, TAKASHI MINAKATA, Asahi Kasei R&D Center, HENNING SIRRINGHAUS, Cavendish Laboratory — We propose a field-induced polymorphous disorder model to explain bias-stress instability in organic pentacene-thin film transistors Field-effect mobility at 0.7 cm²/Vs and threshold voltage, Vth, at 0 V were obtained by using highly crystalline zone-cast pentacene semiconductor on benzyoclobutene insulator. Vth shifted up to +25V with positive gate bias-stress at +40 V for 15 hours and recovered after gate bias removal. Vth recovery was drastically accelerated by direct photo-excitation of pentacene and it indicated electrons were trapped in pentacene and not in BCB. After annealing at 130 °C in N₂, the initial electrical performance were recovered. Micro-Raman spectroscopy of pentacene at the channel revealed that shape of the C-H vibrational peaks at around 1160 cm⁻¹ changed reversibly in accordance with the positive shift and recovery of Vth. Our pentacene films with average d-spacing at 14.3 A were considered to be composed of a mixture (mosaic) of two kind of polymorphs with d-spacing at 14.1 A and 14.5 A. The polymorphous mixture should be disordered by electric field to create electron traps and induce Vth shift.

2:03PM B22.00013 Prediction of the absolute charge mobility of molecular crystals, ALESSANDRO TROISI, University of Warwick — I propose a computational protocol to predict the absolute mobility of molecular semiconductors without adjustable parameters. The system dependent parameters are computed using a combination of classical molecular dynamics simulations and quantum chemical methods. The model used to connect these intractable quantities are the observable temperature dependent mobilities. The model is validated by the accurate prediction of the temperature dependence of the inorganic molecular mobility, and the fluctuation of the transfer integral due to thermal motions. The absolute value of the hole mobility, computed for the case of rubrene, is in excellent agreement with the experiments. The possibility of using computational chemistry methods to improve the theoretical models of charge transfer will be discussed in some detail. The predictive capabilities of the model presented in this work will be further validated considering the recent THz spectroscopy measurements performed by R. van Laarhoven in Eindhoven and the results in literature on temperature dependent band structure and density of state tails.


11:15AM B23.00001 Direct Electron Spectroscopy Investigation of the Spin State of LaCoO₃, J. STANLEY, J. HINTON, N. SUNDARAM, University of California, Santa Cruz, B. S. MUN, A. BOSTWICK, E. ROTENBERG, Lawrence Berkeley National Laboratory, D. P. BELANGER, G.-H. GWEON, University of California, Santa Cruz — The spin state of LaCoO₃ and related properties have been a topic of high interest lately. Here we investigate the electronic structure of LaCoO₃ using core level and valence band photo-electron spectroscopy. We compare the competing spin models in the literature by using our data obtained as a function of incident photon energy and temperature. We are able to make an interesting contribution to the discussion of the spin state of this material.

11:27AM B23.00002 Field Effect on Spin Correlations in La₁₋ₓSrₓCoO₃, DANIEL PHELAN, National Institute of Standards and Technology, DESPINA LOUCA, SEUNGHUN LEE, University of Virginia, STINE ANCONA, STEPHAN ROSENKRANZ, JOHN MITCHELL, Argonne National Laboratory — La₁₋ₓSrₓCoO₃ evolves from a non-magnetic, insulating ground state in the parent compound (x=0) into a metallic, ferromagnetic cluster-glass (x=0.18). For intermediate concentrations, the ground state is characterized by a competition between ferromagnetic and incommensurate spin correlations, which leads to short-range clustering. The field effect on these competing spin correlations has been investigated by neutron diffraction from a single crystal of La₈₅Sr₁₅CoO₃ under an externally applied vertical magnetic field ranging from 0 to 7 T. The intensity of the incommensurate reflections is significantly reduced under 7 T. On the other hand, the ferromagnetic signal is enhanced by more than an order of magnitude under 7 T, while simultaneously narrowing in reciprocal space, implying an increase in the correlation length, which cannot be understood simply by a reorientation of ferromagnetic clusters along the direction of the applied field. Instead, the data is interpreted in a phase-separated scenario in which the applied field polarizes regions which are initially not ferromagnetic in zero field.

11:39AM B23.00003 Ionic Size Effects and Magnetic Incommensurability in Cobaltite, JUAN YU, DESPINA LOUCA, Physics Department, UVA, DANIEL PHELAN, NIST, K. YAMADA, Institute of Materials Research, Tohoku University — LaCoO₃ in which Co⁺⁺ has nearly degenerate spin states shows unusual magnetic behavior attributed to the fact that the different states can co-exist. The cobalt ions interact with each other via complex magnetic coupling, that is further complicated by the addition of Co⁴⁺ ions with hole doping. In the case of hole doped La₁₋₋ₓSrₓCoO₃ (LSCO), we found that the system exhibits a rich phase diagram, dominated by two competing magnetic phases, one that is ferromagnetic and metallic and another that is metallic and incommensurate. Our recent elastic neutron scattering measurements on single crystals of La₁₋₋ₓSrₓBa₂CoO₇ (LBCO) with x = 0.03, 0.06, 0.10 and 0.15) also identified the coexistence of these two phases. Compared to LSCO, the LBCO series shows different incommensurability, but has a similar trend in the progression of intensity with increasing x. However, the LBCO series shows a much longer correlation length particularly in the direction perpendicular to (111), and a significantly stronger incommensurate peak than in LSCO. The incommensurate and ferromagnetic-like intensities exhibit identical temperature dependence in LBCO unlike in LSCO, in which ferromagnetic scattering had a higher onset temperature than the incommensurate phase at identical compositions.

11:51AM B23.00004 Electronic structure of La₁₋₋ₓSrₓCoO₃ investigated from doping evolution of its soft x-ray spectra, YINWAN LI, DAVID EDERER, Tulane University, THOMAS CALLCOTT, University of Tennessee, J. W. FREELAND, Argonne National Laboratory — Pentacite cobalt oxide LaCoO₃ attracted a lot of attention because of its spin state transition around 90K, the interpretation of which is still under debate. We performed soft X-ray absorption and emission experiments on La₁₋₋ₓSrₓCoO₃ at O K-edge and Co L-edge with various doping from x = 0 to x = 30. The doping evolution of the spectra can be understood as a result of introduction of holes at the top of valence band accompanied with a lowering of the Fermi level. The significant change of oxygen K edge spectra with doping indicates that the top of the valence band is largely of oxygen character, indicating strong Co 3d – O 2p hybridization. The bottom of unoccupied band has a double peak feature indicating a splitting e_g band. This split is the largest in the undoped sample and becomes smaller with doping. A gap of less than 1eV is observed from the excitation feature in the emission spectra and its change with doping again indicates a lower Fermi level in doped samples.
12:03PM B23.00005  Thickness dependent magnetotransport properties of epitaxial La$_{0.5}$Sr$_{0.5}$CoO$_3$ (001) films\textsuperscript{1}, M. SHARMA, M. TORJIA, C. LEIGHTON, University of Minnesota, M. VARELA, Oak Ridge National Lab

Thin films of the doped perovskite cobaltite La$_{1-x}$Sr$_x$CoO$_3$ offer an ideal system to study the effect of dimensional confinement on spin state transitions and magnetoelectronic phase separation, and have application possibilities as electrodes in ferroelectric memory and solid oxide fuel cells. In this work we present the magnetotransport properties of epitaxial La$_{0.5}$Sr$_{0.5}$CoO$_3$ (001) thin films deposited on SrTiO$_3$ (001) by high pressure reactive sputtering. The films were structurally characterized by high-resolution x-ray diffraction, scanning probe microscopy, and STEM. Films with thickness > 100 Å exhibit bulk-like ferromagnetic metallic characteristics with the conventional negative MR in the vicinity of T$_C$ and a large AMR at low T. In stark contrast, films with thickness below 60 Å exhibit reduced magnetization and a crossover to an insulating-like temperature dependence of the resistivity. This crossover is accompanied by a large negative MR at low T which bears a striking resemblance to that seen in bulk at x < 0.17, which is known to be due to an intercluster "GMR" effect.

In essence, x = 0.5 films on STO, when sufficiently thin, behave much like x < 0.17 bulk samples, i.e. phase separation is evidenced at the LSCO/STO interface.

\textsuperscript{1}Work supported by NSF DMR and DMSE-DoE.

12:15PM B23.00006  Heat capacity investigation of phase separation and spin-state transitions in La$_{1-x}$Sr$_x$CoO$_3$\textsuperscript{\*}, CHUNYONG HE, University of Minnesota, HENG ZHENG, JOHN MITCHELL, Argonne National Laboratory, C. LEIGHTON, University of Minnesota — We present a heat capacity study (to 0.3 K) on La$_{1-x}$Sr$_x$CoO$_3$ single crystals (0.00 < x < 0.30). In doped samples we observe three contributions at low T; a lattice term (∝ T$^2$), an electronic term (∝ T), and a third term proportional to T$^0$. Remarkably, the x dependence of the electronic and T$^2$ contributions reflects very clearly the known magnetic phase separation, indicating that the T$^2$ term is a signature of the non-F matrix. Possible origins related to AF fluctuations will be discussed. At the lowest T the nuclear hyperfine contribution provides a further probe of magnetic order. The electronic contribution also gives the density of states at the Fermi level which, in combination with the hole density from Hall effect, suggests a large effective mass indicative of strong correlations. Finally, the end-member LaCoO$_3$ shows a striking Schottky anomaly providing new information on the controversial spin-state transition. In particular, we find further evidence of the around 0.5 meV excitation recently observed by inelastic neutron scattering.

\textsuperscript{1}Work supported by DoE and NSF.

12:27PM B23.00007  Phase separation and inhomogeneity in La$_{1-x}$Sr$_x$CoO$_3$ single crystals, W.G. MOULTON, ROBERT SMITH, MICHAEL HOCH, PHILLIP KUHNS, ARNEIL REYES, GREGORY BOBINGER, National High Magnetic Field Laboratory 32310, JOHN MITCHELL, Materials Science Division, Argonne National Laboratory, Argonne, IL, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — Nanoscale inhomogeneity in La$_{1-x}$Sr$_x$CoO$_3$ has been studied in single crystal samples for 0.05 ≤ x ≤ 0.3 using \textsuperscript{139}La NMR as a probe of the internal magnetic field distribution. The results show that phase separation occurs for x near the metal-insulator critical concentration x$_c$=0.17. The phase separation is confined to a much smaller range of x than that previously found in polycrystalline samples even though the bulk magnetic properties are similar. In single crystals with increasing x large, spin polarized (FM) regions merge into networks while smaller regions, identified as spin polarons, coexist with the larger regions. Insight into phase separation has been obtained by simulating the spectra with statistical model A phase diagram summarizing the evolution of the inhomogeneous internal field distribution with x and T will be presented.

12:39PM B23.00008  Strongly Inhomogeneous Conduction in Cobaltite Films\textsuperscript{1}, VLADIMIR ORLYANCHIK, MICHAEL WEISSMAN, UIUC, MÁRIA TORIJA, MANISH SHARMA, CHRIS LEIGHTON, UMN — The prototypical doped perovskite cobaltite, La$_{0.5}$Sr$_{0.5}$CoO$_3$, has received considerable attention in bulk form. It shows a striking Schottky anomaly providing new information on the controversial spin-state transition. It has a ferromagnetic transition at 230 K and an anomalous magnetic transition at 120 K which is manifested in steps in the temperature dependent magnetization and coercivity. The origin of this transition is still under investigation and recent experiments have suggested a change in magnetic anisotropy associated with this anomalous transition. In this work, we report systematic investigations of the magnetic anisotropy and switching fields across the 120 K transition in polycrystalline Pr$_{0.5}$Sr$_{0.5}$CoO$_3$ using a very sensitive RF transverse susceptibility method based on a tunnel diode oscillator resonant at 12 MHz. Our experiments reveal evidence for a sharp change in the anisotropy at 120 K with the anisotropy field (H$^\text{meas}$) dropping from around 1.8 kOe to 750 Oe on cooling. By tracing the evolution of the anisotropy and switching peaks, we are able to discern behavior associated with separate ferromagnetic phases with 120 K signaling the transition between the two.

\textsuperscript{1}This work was funded by NSF DMR 06-05726

12:51PM B23.00009  The spin state issue in the \textit{RBaCo}_2O_5$_{5ь}$ cobaltates, HUA WU, Z. HU, T. BURNUS, D. I. KHOMSKII, L. H. TJENG, Institute of Physics II, University of Cologne, Germany — The double perovskites NbBa$_2$Co$_2$O$_{5ь}$ ($R$=rare earth, 0≤ ν ≤ 1) display intriguing phenomena such as charge and orbital ordering, as well as antiferromagnetic to ferromagnetic transition, depending on the oxygen concentration. In particular, the $\delta$=0.5 system shows a giant magnetoresistance effect, and its metal-insulator transition has been often interpreted in terms of a spin-state transition [1,2], which, however, is fiercely debated [3,4]. To address the spin-state issue, we performed density-functional theory calculations which include a \textit{\emph{\textsuperscript{\*}}}$\delta$-inhomogeneous conductivity may account for the unusual geometry dependent conductance.

1:03PM B23.00010  Magnetic anisotropy and switching in Pr$_{0.5}$Sr$_{0.5}$CoO$_3$ using RF transverse susceptibility\textsuperscript{1}, N.A. FREY, H. SRIKANTH, Physics Department, University of South Florida, D.D. STAUFFER, C. LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota — Pr$_{0.5}$Sr$_{0.5}$CoO$_3$ has been a system of current interest that appears very different from manganites or even other cobaltites. It has a ferromagnetic transition at 230 K and an anomalous magnetic transition at 120 K which is manifested in steps in temperature dependent magnetization and coercivity. The origin of this transition is still under investigation and recent experiments have suggested a change in magnetic anisotropy associated with this anomalous transition. In this work, we report systematic investigations of the magnetic anisotropy and switching fields across the 120 K transition in polycrystalline Pr$_{0.5}$Sr$_{0.5}$CoO$_3$ using a very sensitive RF transverse susceptibility method based on a tunnel diode oscillator resonant at 12 MHz. Our experiments revealed a sharp change in the anisotropy at 120 K with the anisotropy field (H$^\text{meas}$) dropping from around 1.8 kOe to 750 Oe on cooling. By tracing the evolution of the anisotropy and switching peaks, we are able to discern behavior associated with separate ferromagnetic phases with 120 K signaling the transition between the two.

\textsuperscript{1}Work at USF supported by a grant from DOE-BES.
1:15PM B23.00011 Influence of cation and oxygen vacancy ordering on magnetic properties of RE$_{1-x}$Sr$_x$CoO$_{2-\delta}$ (RE=Ho, La) — S. KOLESNIK, B. DABROWSKI, O. CHMAISSEM, J. MAIS, Department of Physics, Northern Illinois University, DeKalb, IL 60115, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, A. BASZCZUK, Institute of Materials Science and Applied Mechanics, Wroclaw University of Technology, 50-370 Wroclaw, Poland — The attractive physical properties of RE$_{1-x}$Sr$_x$CoO$_{2-\delta}$ (RE - rare earth and Y) are strongly dependent upon overall oxygen content $\delta$ and the ordering of oxygen and RE/Sr, as well as charge and spin ordering on the Co$^{3+}$/Co$^{4+}$ sites. Structural, magnetic and thermoelectric properties of Ho$_{1-x}$Sr$_x$CoO$_y$ have been studied within the oxygen content range 2.67<$\delta$<2.80. The studied samples demonstrate antiferromagnetic order (G-type) and semiconductive behavior. No ferromagnetic ordering has been observed and compared with A. Maignan et al. on a closely related Sr$_2$/Y$_{1.5}$/CoO$_5$ with similar $\delta$. We have observed that a the same high degree of oxygen ordering and antiferromagnetic structure exists for both cation disordered (La) and ordered (Y,Ho) materials. We conclude that the high degree of oxygen vacancy ordering determines the observed properties via strong localization of Co$^{3+}$ electrons. Work at NIU was supported by the NSF-DMR-0302617 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

1:27PM B23.00012 Orbital Ordering in Room Temperature Ferromagnet Sr$_3$YCo$_4$O$_{10.5}$ Studied by a Resonant X-ray Scattering — HIRONORI NAKAO, TETSUYA MURATA, DAISUKE BIZEN, YOUICHI MURAKAMI, Tohoku Univ., SHINTARO ISHIWATA, JST-ERATO, WATARU KOBAYASHI, ICHIRO TERASAKI, Waseda Univ. — Sr$_3$YCo$_4$O$_{10.5}$ has been found recently as a room temperature ferromagnet with $T_C$ ~ 340 K, which is the highest $T_C$ among perovskite Co oxides. The crystal structure is formed with the CoO$_6$ octahedral layers and the CoO$_{12.5}$ layers, which stack along c axis alternatively. By powder x-ray diffraction, the orbital state of Co$^{3+}$ (3d$^6$) was evaluated from the anisotropy of the CoO$_6$ octahedron in the ferromagnetic phase, and the $e_g$ orbital ordering of intermediate spin was proposed as an origin of the ferromagnetism. [1] Therefore, the orbital ordering of Co ion has been investigated using a resonant x-ray scattering technique, and a signal resonating near Co K-edge was found clearly. We present an antiferro-orbital and spin-state ordering, and the physical properties can be explained by the ordering model. [1] S. Ishiwata et al., Phys. Rev. B 75 (2007) 220406.

Monday, March 10, 2008 11:15AM - 2:15PM — Session B24 DMP: Focus Session: Transport in Nanostructures II: Strong Correlations Morial Convention Center 216

11:15AM B24.00001 Symmetries and interaction effects in carbon nanotube quantum dots$^1$. GLEB FINKELSTEIN, Duke University — By controlling the contact transparency within the same nanotube quantum dot, we observe the conductance evolving from the well-developed Coulomb blockade through the Kondo regime to the mixed valence regime. We work with high quality nanotubes, where energy subbands are doubly-degenerate, resulting in the SU(4) Kondo effect for one, two, and three electrons filling two degenerate orbitals. As the contacts are made more transparent, the sample enters the mixed valence regime, where different charge states within a pair of orbitals are hybridized. The hallmark of this regime in nanotube conductance is washing out of single-electron features at low temperature. In our measurement the level broadening is close to the charging energy and level spacing (both $\sim$ 10 meV). Nevertheless, the low temperature regime is established only at temperatures of the order or less than 0.5 meV. The same low energy scale is also apparent from the width of the zero-bias peak in the tunneling density of states.

$^1$Supported by NSF DMR-0239748.

11:51AM B24.00002 SU(4) Kondo effect in coupled quantum dots in parallel: Evidence of marginal fixed point$^2$. MIKIO ETO, Keio University — We theoretically study the Kondo effect in coupled quantum dots in parallel, using the scaling and NRG methods. The double quantum dots are capacitively coupled to each other, whereas they are attached to separate leads$^2$. The SU(4) Kondo effect is realized when the energy levels are matched between the quantum dots. We show that (i) the Kondo temperature $T_K$ decreases with increasing $|\Delta|$, where $\Delta$ is the level separation between the dots, obeying a power law [crossover from SU(4) to SU(2) Kondo effect]. (ii) The exponent of the power law is not a universal value in general. This is an evidence of the marginal fixed point of SU(4) Kondo effect$^3$. (iii) The conductance through one of the quantum dots may show a non-monotonic behavior as a function of temperature $T$ although the total conductance is a universal function of $T/T_K$.


12:03PM B24.00003 Exact-diagonalization treatment of the non-universal transport regime in few-electron quantum dots$^1$. LESLIE O. BAKSMATY$^2$, CONSTANTINE YANNOULEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Recently, experimental studies$^3$ have revealed a second transport regime in the behavior of transmission phases obtained via Aharonov-Bohm interferometry using small quantum dots (QDs); namely, a non-universal regime for QDs with $N$ < 10 electrons, in addition to the earlier known universal one for larger QDs with $N$ > 14. Sophisticated (beyond-the-mean-field) many-body methods are needed for describing this non-universal regime. Here, we study the transport properties of small QDs using exact-diagonalization (EXD) calculations in conjunction with Bardeen’s theory of quasiparticle mediated conductance$^4$. We will present EXD calculations$^5$ for anisotropic QDs, and for a wide range of anisotropies and strengths of inter-electron repulsion.

$^1$Supported by the U.S. D.O.E. (FG05-86ER-45234)
$^2$Current address: Physics Dept., Rice University
$^4$For an adaptation of the formalism to QDs, see S.A. Gurvitz, arXiv:0704.1260v1
12:15PM B24.00004 Quantum dot in a Aharonov-Bohm interferometer: magnetic flux-dependent pseudogap in the Kondo regime. — PASCAL SIMON, CNRS and Universite Joseph Fourier, Grenoble, France, LUIS DIAS DA SILVA, Oak Ridge Natl. Lab. and U. of Tennessee, NANCY SANDLER, Ohio University, SERGIO ULLOA, Oak Ridge Natl. Lab. — We study a quantum dot embedded in one of the arms of a Aharonov-Bohm interferometer threaded by a magnetic flux $\Phi$. In the regime where a single resonant mode propagates in the interferometer’s “free arm”, the system can be described by an effective one-channel Anderson impurity model coupled to a non-constant, flux-dependent density of states (DoS). We present numerical renormalization-group results for the Kondo temperature $T_K$, phase shift and finite-temperature linear conductance. For $\Phi \neq 0$, the ground state of the system is Kondo-like, with a renormalized $T_K$. For $\Phi = 0$, the effective DoS vanishes at the Fermi energy and the system maps into the single-particle Anderson model, which displays a quantum critical transition between Kondo and non-Kondo phases [1]. Signatures of these effects appear in the conductance and transmission phase-shifts across the system. This setup constitutes an experimental realization of a tunable pseudogap Anderson Hamiltonian, allowing for an experimental probe into the non-trivial properties of such a model. [1] L.G.G.V. Dias da Silva et al., PRL 97, 096603 (2006).

Supported by NSF-IMC/NIRT.

12:27PM B24.00005 Two-particle processes in quantum dots — ERAN SELA, University of British Colombia — Inelastic two-electron processes in transport through quantum dots can lead to unexpected effects. At the low temperature Kondo regime, transport is described by an effective low-temperature theory in terms of weakly interacting quasiparticles. Despite the weakness of the interaction, we find that the backscattering current and hence the shot noise are dominated by two-quasiparticle scattering. We show that the simultaneous presence of one- and two- quasiparticle scattering results in a universal average charge $5/3e$ as measured by shot-noise experiments. As will be presented, recent experimental data measured in the vicinity of the Kondo limit supports our findings. Furthermore, this experiment suggests that many-body effects are not restricted to the low temperature regime only. Extending our study to the high temperature regime, we found under general conditions in Coulomb blocked quantum dots, signatures of transfer of electron pairs. Those results on many-body corrections to the cotunneling current will be discussed in a related talk by M.E. Raikh.

1:03PM B24.00006 ABSTRACT WITHDRAWN

1:15PM B24.00007 Finite-temperature conductance signatures of a quantum-critical transition in a double quantum-dot device — NANCY SANDLER, Ohio University, LUIS DIAS DA SILVA, Oak Ridge Natl. Lab. and U. of Tennessee, KEVIN INGERSENT, U. of Florida, SERGIO ULLOA, Ohio University — We present conductance results for a quantum-dot system containing one dot in the Kondo regime coupled to two leads in parallel with a noninteracting resonant level. The system can be mapped onto a single-impurity Anderson model with a pseudogapped effective density of states [1]. The finite-temperature linear conductance $G(T)$ of this double-dot device is obtained via numerical renormalization-group calculations. The position of the single-particle levels can be controlled with gate voltages so that the effective density of states vanishes in power-law fashion at the Fermi energy of the leads; within this regime, further tuning can drive the system through a quantum critical point separating Kondo and unscreened phases. Signatures of both effects appear in $G(T)$, with a prominent feature at the scale $T^*$ marking the crossover from the high-temperature quantum-critical regime to a low-temperature Fermi liquid. These results open the way for experimental verification of the effect, and in principle allow access to a quantum critical point in a unique tunable system. [1] L.G.G.V. Dias da Silva et al., PRL 97, 096603 (2006).

Supported in part by NSF DMR-0312939 and NSF-IMC/NIRT.

1:27PM B24.00008 Conductance signatures of quantum phase transitions in asymmetric double quantum dots — W. BRIAN LANE, Jacksonville U. and U. of Florida, KEVIN INGERSENT, U. of Florida, LUIS DIAS DA SILVA, Oak Ridge Natl. Lab. and U. of Tennessee, NANCY SANDLER, SERGIO ULLOA, Ohio U. — Double quantum dots (DQDs) are currently of great theoretical and experimental interest. A DQD device in which dot 1 is in the Kondo regime and dot 2 acts as a noninteracting resonant level can be tuned to access a pair of quantum phase transitions separating Kondo-screened and local-moment phases [1]. This talk focuses on the effects of introducing a nonzero Coulomb interaction $U_2$ on the second dot. For small $U_2$, the system continues to exhibit two quantum phase transitions, although their nature is markedly different than for $U_2 = 0$. However, stronger interactions $U_2 > U_1$ suppress the local-moment phase and destroy the quantum phase transitions. We use numerical renormalization-group techniques to identify signatures of these behaviors in the linear conductance of the DQD device. [1] L. G. V. Dias da Silva, N. P. Sandler, K. Ingersent, and S. E. Ulloa, Phys. Rev. Lett. 97, 096603 (2006).

Supported by NSF Grants DMR-0312939 and DMR-0710540 (Florida), DMR-0304314 and DMR-0710581 (Ohio).

1:39PM B24.00009 Symmetries and conductance in Kondo quantum dots — EDSON VERNEK, CARLOS BÜSSER, Ohio University, ENRIQUE V. ANDA, PUC-Rio, Brasil, NANCY SANDLER, SERGIO E. ULLOA, Ohio University — The role of symmetries on nanoscale structures is essential for the physical behavior exhibited in these systems while its understanding offers deeper insights into the observed properties. The ability to fabricate structures such as quantum dot arrays with tailored symmetries provides further motivation to understand the interplay of geometrical and orbital symmetries in interacting systems at low temperatures, where quantum coherence and Kondo correlations determine the electronic properties. In this work we study the transport properties of three interconnected quantum dots coupled to different leads in a triangular geometry. Conductance calculations carried out in a finite-U slave-boson mean field approximation show excellent agreement with results from the embedded cluster approximation (ECA), highlighting the rich features of the various physical regimes. We focus on and compare two important geometries with: equilateral (all couplings and leads identical) and isoceles (one lead and respective couplings different from the others) symmetries. In the first case, we show that only two degenerate orbitals contribute to the Kondo state conductance. Further, we show that the presence of an open third lead in all cases introduces dephasing which affects differently the various features of the conductance.

1:51PM B24.00010 Kondo correlations and transport in single and triple quantum dots with damped lead hoppings: a tDMRG study — LUIS DIAS DA SILVA, Oak Ridge Natl. Lab. and U. of Tennessee, FABIAN HEIDRICH-MEISNER, Inst. for Theoretical Physics C, RWTH Aachen, Germany, ADRIAN FEIGUIN, Microsoft Project Q, U. of California at Santa Barbara, ELBIO DAGOTTO, Oak Ridge Natl. Lab. and U. of Tennessee — We study the transport properties of one and three quantum dot systems with the time-dependent Density Matrix Renormalization-Group method (tDMRG). As previously noted [1,2], fine-size effects make the tDMRG description of the strongly interacting Kondo regime a numerically demanding task. We address this issue by introducing an exponential decay in the hopping terms in the leads ($t_{ij} \propto \lambda^{-n/2}$), recently introduced in cluster embedding methods [3]. For a given size system, results for $\lambda > 1$ show several improvements over the undamped ($\lambda = 1$)[1,2] case: the Kondo plateau in the differential conductance is correctly obtained deeper in the strongly interacting regime; steady-state current plateaus remain well defined for longer time scales. These results show that, with the proposed modification, the characterization of Kondo correlations in the transport properties can be substantially improved, at less computational cost. [1] K. A. Al-Hassanieh et al. PRB, 73, 195304 (2006). [2] F. Heidrich-Meisner et al. arxiv:0705.1801 (2007). [3] E. Anda et al., pre-print (Nov. 2007).

Sponsored in part by NSF grant DMR-0706020 and U.S. DOE.
NB controlled not only by the degree of polymerization of the surrounding linear chains, but also by the degree of polymerization of the brush's side chains, \( \chi(T) \). In simulations of simple models, a useful independent definition of \( \chi(T) \) may be obtained from a thermodynamic perturbation theory in which the difference between AB and AA interactions is treated as a perturbation of a one-component melt. For lattice models, this yields a value that, in the limit of long chains, is related to the Flory-Huggins value by replacing the coordination number \( z \) by an effective coordination number given by the average number of inter-molecular contacts per monomer, as proposed previously by M. Mueller. Generalizations of the idea are provided for continuum models, and for shorter chains. An analytic theory is presented that quantitatively predicts the N-dependence of the effective coordination number found in lattice simulations. The approach provides a clean way to separate RPA from non-RPA effects in the analysis of simulations.

**Monday, March 10, 2008 11:15AM - 2:03PM**

**Session B25 DPOLY: Polymer Blends** Marriot Convention Center 217

**11:15AM B25.00001 Effective Coordination Number and Interaction Parameter In Simple Models of Polymer Blends** DAVID MORSE, University of Minnesota — One challenge faced when trying to quantify corrections to the RPA in either simulations or experimental measurements of correlations in polymer blends is the need to estimate the temperature or parameter dependence of a self-consistent field interaction parameter \( \chi(T) \). In simulations of simple models, a useful independent definition of \( \chi(T) \) may be obtained from a thermodynamic perturbation theory in which the difference between AB and AA interactions is treated as a perturbation of a one-component melt. For lattice models, this yields a value that, in the limit of long chains, is related to the Flory-Huggins value by replacing the coordination number \( z \) by an effective coordination number given by the average number of inter-molecular contacts per monomer, as proposed previously by M. Mueller. Generalizations of the idea are provided for continuum models, and for shorter chains. An analytic theory is presented that quantitatively predicts the N-dependence of the effective coordination number found in lattice simulations. The approach provides a clean way to separate RPA from non-RPA effects in the analysis of simulations.

**11:27AM B25.00002 Nucleation in Polymer Blends** EDWARD FENG, NITASH BALSARA, University of California, Berkeley — Balsara and co-workers used small angle neutron scattering experiments on binary homopolymers blends to determine the size of the critical nucleus during phase separation. This suggests measuring the size of a single critical nucleus through a measurement of total density fluctuations. We carefully analyze this idea through kinetic Monte Carlo simulations of the Ising model, performing simulations of phase separation that conserve and do not conserve the magnetization. Calculations of the structure factor and spin-spin correlation function reveal clear differences in the nucleation mechanism for these two dynamics. Simulations that conserve the magnetization qualitatively agree with the experimental results on binary blends. Moreover, we calculate the cluster distribution during nucleation to determine the critical nucleus size of the Ising model. Comparing this result with the value determined from the structure factor shows qualitative agreement with increasing supersaturation.

**11:39AM B25.00003 Molecular dynamics simulations of constraint release effects in entangled binary blends of linear polymers** ZUOWEI WANG, RONALD G. LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109-2136 — We present extensive molecular dynamics simulations of the dynamics of entangled binary blends consisting of long test chains diluted in shorter chain matrix. The ratio between the long and short chain lengths is varied by a factor of ten covering the crossover from the chain reptation regime to the tube Rouse relaxation regime. Consistent with Neutron Spin Echo experiments, the dynamic structure factor of the long chains is found to decay faster in the matrix with shorter chain lengths, owing to the stronger constraint release effect. Correspondingly the monomers and centers of mass of the long chains show a faster time-dependent diffusivity than that expected from pure reptation. The simulation results for the diffusion properties agree qualitatively with the predictions based on constraint release Rouse motion model at long time scales, but show deviations from the theoretical predictions in the intermediate time regime. Our preliminary analysis of diffusion of the matrix chains in the tube-region of the long chains indicates that this discrepancy results from neglect of the broad distribution of the lifetimes of constraint release events in the theoretical treatment.

**11:51AM B25.00004 Flory Theorem for Structurally Asymmetric Mixtures** ANDREY DOBRYNIN, Institute of Materials Science, University of Connecticut, FRANK SUN, DAVID SHIRVANYANTS, GREGORY RUBINSTEIN, MICHAEL RUBINSTEIN, SEUNG-JUN HEO, Department of Chemistry, University of North Carolina at Chapel Hill, HYUNG-IL LEE, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University — The generalization of the Flory theorem for structurally asymmetric mixtures was derived and tested by direct visualization of conformational transformations of brushlike macromolecules embedded in a melt of linear chains. Swelling of a brush molecule was shown to be controlled not only by the degree of polymerization of the surrounding linear chains, \( NB \), but also by the degree of polymerization of the brush’s side chains, \( N \), which determines the structural asymmetry of the mixed species. The boundaries of the swelling region were established by scaling analysis as \( N^{2/3} < NB < NA/N \), where \( NA \) is the degree of polymerization of the brush backbone. Experiment and theory demonstrated good agreement.

**12:03PM B25.00005 The Molecular Weight and Composition Dependence of Measured Flory-Huggins Interaction Parameters for Blends of Model Polyolefins** ALISYN NEDOMA, Univ. of California, Berkeley, MEGAN ROBERTSON, Univ. of Minnesota, NISITA WANAKULE, NITASH BALSARA, Univ. of California, Berkeley — The thermodynamics of binary blends of model polyolefins (deuterated polybutadiene and polysisobutylene) was studied using small angle neutron scattering (SANS) and small angle light scattering (SALS). SANS experiments on single phase blends reveal that the Flory-Huggins interaction parameter, \( \chi_i \), for this system depends on both blend composition and component molecular weights. This is in contrast to numerous previous studies on thermodynamics of polymer blends where \( \chi_i \) is reported to be independent of molecular weight. The phase separation temperatures of our blends, determined by SALS and SANS, will be compared to predictions based on the measured \( \chi_i \) parameters.

We acknowledge the support of the National Institute of Standards and Technology, U.S. Department of Commerce, in providing the neutron research facilities used in this work.

**12:15PM B25.00006 Porod SAXS Studies of Shear-Induced Droplet Deformation in a Concentrated Immiscible Polymer Blend** WESLEY BURGHARDT, KRISTIN BRINKER, Northwestern University — Droplet deformation, break-up and coalescence of immiscible polymer blends under flow is fundamental to understanding the effect of processing on ultimate blend properties, as well as the excess rheological properties associated with deformation of the multiphase structure. Both optical methods have frequently been employed to gain insight into these processes, but in most cases, optical methods are restricted to quite dilute concentrations, owing to concerns of high turbidity and multiple scattering. Here we explore used of time-resolved synchrotron small-angle x-ray scattering as an alternative method to study multiphase materials under shear. Typical blend droplet sizes of ~1 micron are large relative to length scales typically probed by SAXS; however, the wide-angle limit of small-angle scattering (i.e. the Porod regime) is directly sensitive to interfacial structure of multiphase materials and, when rendered anisotropic by shear flow, provides direct insights into the deformation and orientation of interface. We report scattering studies in the flow-gradient plane of a polystyrene/polymethyl methacrylate) blend, which is approximately viscosity matched, to step-strain deformations. Postulating that each droplet is deformed to a geometrically similar shape, data are analyzed in the context of a model of Porod scattering from ellipsoids.
12:27PM B25.00007 Measurements of the Onsager coefficient in a phase-separating polymer blend, AMISH PATEL, NITASH BALSARA, U. C. Berkeley — Phase separation in a polymer blend of critical concentration was studied using time-resolved Small Angle Neutron Scattering (SANS). To start off, the blend was homogenized by taking it well into the 1-phase region of the phase diagram. It was then quenched into the 2-phase region by using a rapid change in pressure. Since, the sample enters the two-phase region at the critical point, it is expected to phase separate by spinodal decomposition. Hence, the time dependent SANS intensity was fit to the Cahn-Hilliard-Cook equation for systems undergoing spinodal decomposition. The fit parameters were then used to calculate the non-local Onsager coefficient at several different pressures. The functional form of the Onsager coefficient, as a function of the wave-vector, was compared to that predicted by theory. Finally, the molecular parameters that go into the theory were extracted.

12:39PM B25.00008 Structure And Dynamics Of Semi-crystalline Polyethylene Oxide / Polyvinyl Acetate Blends 1, JAMES RUNT, DANIEL FRAGIADAKIS, Penn State University — The structure and dynamics of semi-crystalline, melt-miscible polyethylene oxide / polyvinyl acetate (PEO/PVAc) blends were investigated using small-angle X-ray scattering and dielectric relaxation spectroscopy. PEO/PVAc blends with selected compositions were crystallized at various temperatures. Small-angle X-ray scattering was used to quantitatively determine the semi-crystalline microstructure, including the location(s) of the non-crystallizable PVAc in the structure. Segmental and local dynamics were studied using broadband dielectric relaxation spectroscopy. We attempt to clarify the origin of an additional relaxation, located at intermediate frequencies between the segmental and local processes, which has been proposed to be related to initial stages of crystallization even in blends lacking macroscopic crystallinity.

1Supported by the NSF Pioneers Program, DMR-0605627

12:51PM B25.00009 The Structure and Thermodynamics of Cellulose Acetates, MARK DADMUN, RUJUL MEHTA, University of Tennessee, GARY LYNN, Oak Ridge National Laboratory — Cellulose acetate (CA) polymers having different degrees of substitution (DS) vary widely in their properties, such as glass transition, miscibility, chemical resistance, and gas permeation. These variations hint at differences in their molecular structure. We have systematically studied the variation in the molecular structure of CA with DS, utilizing small angle neutron scattering (SANS). SANS measurements were carried out in 1% (w/v) solutions in DMSO (which is sufficiently dilute to avoid intermolecular scattering). The polymer chains display rigidity along their main chain and have persistence lengths in the range of 12 to 14 nm. The effect of DS on the extent of miscibility is explained on the basis of available intra-molecular hydrogen bonding sites along the polymer chain. SANS measurements were also carried out on 50-50(w/w) miscible blends of two sets of CA, where the difference in the DS between the polymers varied from 0.05 to 0.25. Random phase approximation analysis provides an estimate of the Flory-Huggins interaction parameter between the two polymers in the blend. The influence of both the amount of substitution and hydrogen bonding on the polymer miscibility will be discussed.

1:03PM B25.00010 Effect of solvent evaporation and coagulation on morphology development of asymmetric membranes, NEELAKANDAN CHANDRASEKARAN, THEIN KYU, The University of Akron — Miscibility behavior of blends of amorphous polycarbonate (PA) and polyvinylpyrrolidone (PVP) was studied in relation to membrane formation. Dimethylsulfoxide (DMSO) and water were used as solvent and non-solvent, respectively. Differential scanning calorimetry and cloud point measurements revealed that the binary PA/PVP blends as well as the ternary PA/PVP/DMSO system were completely miscible at all compositions. However, the addition of non-solvent (water) to this ternary system has led to phase separation. Visual turbidity study was used to establish a ternary liquid-liquid phase diagram of the PA-PVP/DMSO/water system. Scanning Electron Microscopy (SEM) showed the development of finger-like and sponge-like cross sectional morphologies during coagulation. Effects of polymer concentration, PA/PVP blend ratio, solvent/non-solvent quality, and evaporation time on the resulting membrane morphology will be discussed.

1:15PM B25.00011 The Glass Transition and Dynamics in Athermal Poly(a-Methyl Styrene)/Oligomer Blends, WEI ZHENG, SINDEE SIMON, Texas Tech University — The glass transition and dynamics in athermal blends of poly(a-methyl styrene) (PMS) and its short chain oligomers are investigated using differential scanning calorimetry (DSC). A methodology is described to partition the calorimetric transition in order to obtain effective Tgs for each component of the blend. The dependences of these effective Tgs on overall blend composition are described by the Lodge-McLeish model although the self-concentration effect is less than expected based on the Kuhn length. The kinetics associated with the glass transition, Tg, are examined by studying the cooling rate dependence of Tg for the pure components and the blends, as well as by examining the enthalpy overshoots in the heating DSC scans. Extension of Colmenero’s model to describe the dynamics in these materials will be discussed.

1:27PM B25.00012 Effect of compositional heterogeneity on the phase structure and crystallization behavior of polypropylene in-reactor alloys, DUJIN WANG, HAIJIN ZHU, BENJAMIN MONRABAL, CHARLES C. HAN — Although the compositional heterogeneity and chain structure of PP/EPR in-situ blends have been extensively investigated, little is known about the conclusive relationship among the molecular/phase structure and the ultimate mechanical properties due to its complex compositions in such systems. A systematic study was conducted on the compositional heterogeneity, phase structure, the crystallization and subsequent melting behavior of two in-reactor alloys EB-P and EP-P. The composition of the alloys and the chain structure of each component were characterized by preparative TREF and 13C-NMR technique. The results showed that the excellent balance between toughness and rigidity of EB-P primarily benefits from the polyethylene homopolymer (HE) phase and the ethylene-o-cycloolefin copolymer (EC) component, which is enriched at the interface between the dispersed phase (HPP) and the matrix (HE). As for EP-P, the amorphous EC and the interpenetrating phase are mainly responsible for the outstanding low temperature impact toughness.

1Financial support from Ministry of Science and Technology is greatly acknowledged.

1:39PM B25.00013 Mesoscopic drop dynamics and rheological modeling for polymer blends, YUANZE XU, Fudan University, WEI YU, Shanghai Jiao Tong University, JIANMAO YANG, Fudan University — Fundamental challenge to rheology for polyblends originates from the dynamic coupling between interfacial morphology and viscoelastic flow. This work will outline our approaches. The framework of irreversible thermodynamics was employed to model immiscible viscoelastic blends considering the chain conformation, the drop deformation, drop break-up and collapse and the hydrodynamic interaction of drops in concentrated blends. The theoretical predictions were proved by measuring the drop dynamics in a four-roll mill rheometer with success. Great challenge to the model exists in systems where the drop dynamics severely deviating from emulsions of Newtonian droplets. A new type of drop merging by a string pulling two beads together (BSB) was observed and analyzed. The relevant material and process conditions causing BSB or beads-on-string are discussed elucidating its origin of non-linear viscoelasticity of polymers.

1NSF-China Key Proj. 20490224
1:51PM B25.00014 Self Similar Growth of Polyolefin Blends On a Micro-Nano Granule Reactor

CHARLES HAN, JIANG DU, KUN MENG, XIA DONG, JIN-YONG DONG,1 DUSJIN WANG, State Key Laboratory of Polymer Physics and Chemistry, Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China — A Ziegler-Natta/metalocene hybrid catalyst was used in this MRGT (Multi-catalyst Reactor Granule Technology) synthesis. Isotactic polypropylene/polyethylene-co-octene (iPP/PEO) polymer blends were prepared on the micro-nano granule reactors. A self-similar growth mechanism has been observed and deciphered. The self-similar structure is extended and observed at least for 5 decades in a combined real and reciprocal spatial range. With thermal treatment, structure growth and crystallization kinetics has been studied on these single reactor granules.

Monday, March 10, 2008 11:15AM - 2:15PM –
Session B26 DCP: Focus Session: Photophysics of Cold Molecules II
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11:15AM B26.00001 Molecular collision studies with Stark-decelerated beams, GERARD MEIJER, Fritz-Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany — Molecular scattering behaviour has generally proven difficult to study at low collision energies. We formed a molecular beam of OH radicals with a narrow velocity distribution and a tunable velocity by passing the beam through a Stark decelerator [1]. The transition probabilities for inelastic scattering of the OH radicals with Xe atoms were measured as a function of the collision energy in the range of 50 to 400 wavenumbers. The behaviour of the cross-sections for inelastic scattering near the energetic thresholds was accurately measured, and excellent agreement was obtained with cross-sections derived from coupled-channel calculations on ab initio computed potential energy surfaces [2]. For collision studies at lower energies, the decelerated beams of molecules can be loaded into a variety of traps. In these traps, electric fields are used to keep the molecules confined in a region of space where they can be studied in complete isolation from the (hot) environment. Typically, 107 state-selected molecules can be trapped for times up to several seconds at a density of 107 mol/cm3 and at a temperature of several tens of mK [3]. The long interaction time afforded by the trap has been exploited to measure the infrared radiative lifetime of vibrationally excited OH radicals, for instance, as well as to study the far-infrared optical pumping of these polar molecules due to blackbody radiation [4]. As an alternative to these traps, we have demonstrated an electrostatic storage ring for neutral molecules. In its simplest form, a storage ring is a trap in which the molecules - rather than having a minimum potential energy at a single location in space - have a minimum potential energy on a circle. To fully exploit the possibilities offered by a ring structure, it is imperative that the molecules remain in a bunch as they revolve around the ring. This ensures a high density of stored molecules, moreover, this makes it possible to inject multiple - either co-linear or counter propagating - packets into the ring without affecting the packet(s) already stored. We have recently demonstrated a prototype molecular synchrotron, which will be used as a low-energy collider for neutral molecules in the future [5].


11:51AM B26.00002 Magnetoelectrostatic trapping of neutral OH molecules1, BRIAN SAWYER, BENJAMIN STUHL, JILA/University of Colorado, BENJAMIN LEV, University of Illinois, Urbana-Champaign, MARK YEO, JILA/University of Colorado, D AJUN WANG, JUN YE, JILA/NIST/University of Colorado — Advances in cold molecule production promise to profoundly impact research on precision measurement, quantum information, and controlled chemistry. To this end, we employ a Stark decelerator to remove 99.5% of the center-of-mass kinetic energy of a super-bunch as they revolve around the ring. This ensures a high density of stored molecules, moreover, this makes it possible to inject multiple - either co-linear or counter propagating - packets into the ring without affecting the packet(s) already stored. We have recently demonstrated a prototype molecular synchrotron, which will be used as a low-energy collider for neutral molecules in the future [5].

[1] The authors acknowledge support from the NSF, DOE, NIST, and NRC.

12:03PM B26.00003 Photodissociation of SO2 as a way to cold atoms and molecules, LISDAT CHRISTIAN, Physikalisches-Technische Bundesanstalt, Braunschweig, Germany, OLEG BUCICOV, MARCIN NOWAK, SEBASTIAN JUNG1, EBERHARD TIE-MANN, Institute of Quantum Optics, Leibniz University Hannover, Germany — We discuss the possibility of using the photodissociation of cold SO2 molecules to produce internally and translationally cold photofragments SO and O. It is expected from our measurements of the molecular Stark effect [1] that the dissociation pathways and excess energies of the fragments are tunable by electric fields [2]. Cold SO2 molecules are produced by Stark deceleration. We have realized a Stark decelerator that is able to slow down packages SO2 in weak-field seeking levels to a few 10 m/s center of mass velocity. A Stark decelerator with 326 stages is required for this purpose, since the ratio of Stark shift to initial kinetic energy is small for SO2. The photofragments SO and O have triplet ground states, while the ground state of SO2 is diamagnetic. In combination with the photodissociation at the threshold we want to employ this constellation to accumulate fragments in a magnetic trap by dissociating SO2 as it is stopped by electric fields in the center of the trap.


1present address: Atomic Physics Division, NIST Gaithersburg

12:15PM B26.00004 Alternating gradient focusing and deceleration of large molecules, KIRSTIN WOHLFART, FABIAN GRÄTZ, FRANK FILSINGER, GERARD MEIJER, JOCHEN KÜPPER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — During the last decade, fascinating progress has been made in the spectroscopy of the “molecular building blocks of life”. Meanwhile, our group has been developing methods to decelerate neutral, polar molecules using time varying inhomogeneous electric fields. Extending these techniques to bio-molecules would allow, for instance, to increase observation times for precision spectroscopy or to separate different conformers. However, for such large molecules all states are practically high-field seeking. Therefore, alternating gradient focusing has to be applied. Here, we demonstrate the focusing and deceleration of benzonitrile (C6H5N) from a molecular beam. Benzonitrile is prototypical for large asymmetric top molecules that exhibits rich rotational structure and a high density of states. It is decelerated in its absolute ground state from 320 m/s to 289 m/s, and similar velocity changes are obtained for excited rotational states. We are setting up a longer alternating gradient decelerator, which will enable us to decelerate benzonitrile or larger molecules to much lower velocities and to thereby completely separate the decelerated packet from the rest of the beam pulse.
1:15PM B26.00007 Kinetics of Cold Molecule Production in “Kinematic” Cooling , JEFFREY KAY, KEVIN STRECKER, DAVID CHANDLER, Sandia National Laboratories — “Kinematic” cooling is a general technique by which a vast array of molecules can be translationally cooled using crossed atomic and molecular beams. The success of the technique relies primarily on the existence of an approximate mass degeneracy between the molecule to be cooled and its atomic or molecular collision partner. Here, we discuss factors that affect the efficiency of cold molecule production by this method, as well as schemes that may allow tunability of the velocity and temperature of the cold molecules on a fine scale.

1:27PM B26.00008 A new source for quantum optics with biomolecules and biomolecular clusters , MARKUS MARKSTEINER, PHILIPP HASLINGER, HENDRIK ULBRICH, MARKUS ARNDT, Faculty of Physics, University Vienna — We present recent progress towards matter wave experiments with amino acids, polypeptides and large biomolecular clusters. All successful experiments on macromolecule interferometry so far, with fullerenes, fullerene derivatives and large perfluoroalkyl-functionalized azobenzenes used effusive beam sources. The combination of Stark deflection with quantum interferometry also allowed us to create a new device for precisely measuring electric susceptibilities of large molecules in the gas phase. In order to apply quantum interference to molecules of biological interest, we have now implemented a pulsed laser desorption source. The combination of UV laser desorption into an intense noble gas jet and single-photon ionization by a VUV excimer laser (157nm) allows us to observe intense neutral jets of amino acids (e.g. Tryptophan), nucleotides (e.g. Guanin) and polypeptides ranging from tri-peptides to Gramicidin. Remarkably, we also found a new method for producing large neutral amino acid clusters, such as for instance Trp$_{30}$, with masses exceeding 6000 amu: the addition of alkaline Earth salts in the desorption process leads to the inclusion of at least one metal atom per complex and is sufficient to catalyze the cluster formation process.

1:39PM B26.00009 Collisions of ultracold molecules , HANNS-CHRISTOPH NAEGERL, University of Innsbruck — In our experiments we routinely produce ultracold trapped samples of dimer molecules out of a Cs atomic gas by exploiting the atom-dimer coupling near Feshbach resonances. We explore the rich molecular structure for the Cs dimers near the atomic threshold by consecutive state transfer after initial dimer production and produce atom-dimer mixtures for which we measure the atom-dimer collisional rate as a function of kinetic energy at temperatures down to 40 nK. We find resonant enhancement of this rate for sufficiently small dimer binding energies for which coupling to an Efimov trimer state is possible. We also produce pure dimer samples for which we measure the collisional loss rate. For a weakly bound molecular s-state this rate depends strongly on temperature and on the applied magnetic field. We will also discuss first results from our experiment on producing ultracold ro-vibrational ground state molecules for the case of Cs dimers and RbCs starting from weakly bound molecules which initially are produced on a Feshbach resonance.

Monday, March 10, 2008 11:15AM - 2:15PM — Session B27 GMAG: Focus Session: Molecular Magnets I Morial Convention Center 219

11:15AM B27.00001 Self-Assembled Growth and Magnetism of Ordered Cluster Arrays , AXEL ENDERS, University of Nebraska - Lincoln — It is generally recognized that the fabrication of magnetic storage media with bit densities of Gigabytes per square inch and more is out of reach of currently available thin film technologies. Patterned media may therefore set off to challenge thin film media as they allow in principle for bit densities several orders of magnitude larger than what is currently feasible. In this talk I will show how nanoclusters can be fabricated on substrates directly by self-assembled growth, and how their magnetism and their lateral arrangement on the substrate can be controlled. Buffer layer assisted growth is used to form clusters of controlled density and size, in the range between a few atoms to several nanometers diameter. The clusters are randomly distributed over the bare substrate surface. The cluster nucleation on the buffer layer and their growth after making contact with the substrate was studied with variable temperature scanning tunneling microscopy, and will be discussed in the talk. The investigation of the cluster magnetism with X-ray magnetic circular dichroism revealed size and strain effects as well as mutual dipolar and cluster-substrate interactions. We found a pronounced dependence of the magnetic anisotropy on the substrate material. On Pt, for instance, the preferential magnetization direction is out-of-plane, while it is in-plane on Ag. The application of self-assembled clusters as individually addressable magnetic units requires their controlled arrangement into well-defined ordered arrays. We are therefore guiding the clusters with energetic sinks provided by periodic network structures prefabricated on the substrate. We use mechanically extremely stable, electronically insulating boron nitride nanomesh monolayers as template surfaces. Repeated cluster deposition cycles increase the cluster density on the nanomesh, eventually resulting in an densely packed, ordered cluster array with a cluster-cluster distance corresponding to the BN nanomesh periodicity of 3.2 nm. These cluster layers offer densities of magnetic elements as high as 80 x 10$^{12}$ clusters per square inch.

11:51AM B27.00002 Transition linewidth of Mn12-Acetate$^1$, BETH PARKS, KURT ANDRESEN, Colgate University, CHRISTOPHER BEEDLE, DAVID HENDRICKSON, UC San Diego — The single-molecule magnet Mn$_{12}$-acetate forms macroscopic crystals in which quantum tunneling of the magnetic moment can be observed. This quantum tunneling is governed to a large extent by defects in the crystal structure. These same defects are thought to be responsible for the broadening of the transition linewidth between adjacent levels, such as $m_s = 10$ to $m_s = 9$. It is possible to test this understanding by observing the linewidth of the transition during the tunneling process. If the same defects are responsible for both effects, then as tunneling progresses, the linewidth should change. Results of this measurement of the linewidth obtained using terahertz time-domain spectroscopy will be presented.

$^1$This research was supported by the National Science Foundation.
12:03PM B27.00003 Low temperature relaxation crossover in one dimensional chain-like molecular magnet \([\text{Fe}^\text{II}(\Delta)\text{Fe}^\text{II}(\Lambda)\text{(ox)}_2(\text{phen})_2]_n\) , J.L. HER, C.P. SUN, S. TARAN, C.C. CHOU, C.L. CHAN, C.C. LIN, Department of Physics, Center of Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, L.L. LI, K.J. LIN, Department of Chemistry, Center of Nanoscience and Nanotechnology, National Chung-Hsing University, Taichung 402, Taiwan, H.D. YANG, Department of Physics, Center of Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The frequency-dependent ac susceptibility, theromromagnetization magnetization relaxation (TRM) and magnetic field dependent magnetization have performed on a hand-aligned partially orientated molecular magnet compound \([\text{Fe}^\text{II}(\Delta)\text{Fe}^\text{II}(\Lambda)(\text{ox})_2(\text{phen})_2]_n[\text{I}]\) which exhibits one dimension chain like structure. The ac susceptibility shows spin glass-like relaxation at temperatures between 7.8 and 8.2 K. In addition, the TRM results show various relaxation behaviors below \(T_m \sim 8.6\) K, indicating that there is a remnant instability at low temperature. It might be caused by the complex interaction within and/or between the chains and the stacked layers. With slowly sweeping the magnetic field, a step-like behavior in the magnetic hysteresis loop was observed below \(T_m\). The possible origins for these properties are discussed. [1] L. L. Li, K. J. Lin, C. J. Ho, C. P. Sun, and H. D. Yang, Chem. Commun. 12, 1286 (2006).

12:15PM B27.00004 A novel experiment using rotating magnetic fields to study the pumping spin states in molecular magnets , ALBERTO HERNANDEZ-MINGUEZ, FERRAN MACIA, JOAN MANEL HERNANDEZ, CARLA CARBONELL, ROGER AMIGÓ, JAVIER TEJADA, Universitat de Barcelona — We report here a new experimental technique to monitor spin population dynamics in molecular magnets. This deals with a huge rotating magnetic field initially applied along the easy magnetization direction, \(z\)-axis, that rotates with components parallel and perpendicular to the \(z\) axis. This technique allows us to probe spin relaxation on reasonably fast time scales detecting the inversion of the whole spin states. The population of spin levels depends on the frequency of the rotating magnetic field. This very new technique could help to carry out new experiments in a number of different fields, broadening substantially the scope of their use until now. A Hernández-Minguez et al., Appl. Phys. Lett. 91, 202502 (2007).

12:27PM B27.00005 Anomalous magnetic relaxation in 2D layered organic-based magnet \([\text{Fe(TCNE)(NCMe)}_2][\text{FeCl}_4]\) , JUNG-WOO YOO, V. N. PRIGODIN, Department of Physics, The Ohio State University, K. I. POKHOD-NYA, JOEL S. MILLER, Department of Chemistry, University of Utah, A. J. EPSTEIN, Department of Physics and Chemistry, The Ohio State University — The magnetic relaxation of the 2D organic-based magnet \([\text{Fe(TCNE)(NCMe)}_2][\text{FeCl}_4]\) was explored using both static and dynamic measurements. Static \(M(H,T)\) studies showed that the ferrimagnetic order between the spins in \(\text{Fe}^\text{II}\) \((S = 2)\) and the spin in \((\text{TCNE})^-\) \((S = 1/2)\) occurs principally within the plane of \([\text{Fe(TCNE)(NCMe)}_2]\) layers, with no magnetic coupling to the \(S = 5/2\) of the \([\text{FeCl}_4]^-\), which is located between layers [1]. The DC magnetic relaxation in ZFC states shows the memory effects similar to that observed in superparamagnetic systems. This reflects the weak magnetic coupling between the layers enabling the bistable nature between FC and ZFC states [1]. The memory effects disappear when the system is cooled in field supporting bistable nature of interlayer coupling. The dynamic susceptibility near the critical \(T\) shows two relaxation processes the possible origins of which will be discussed. [1] K. I. Pokhodnya, et al. J. Am. Chem. Soc., 118, 12844 (2006).

12:39PM B27.00006 Ferromagnetic resonance (FMR) of a room temperature organic based mixed valent Vanadium Hexacyanochromate magnet \(K_{1.54}\text{V}^{\text{III}}\text{V}^{\text{II}}\text{V}^{\text{III}}\text{Cr}^{\text{III}}\text{(CN)}_6\text{(SO}_4\text{)}_{0.16}\text{3.1H}_2\text{O}\) , N.P. RAJU, J.W. YOO, Dept. of Physics, The Ohio State University, AMBER C. MCCONNELL, WILLIAM W. SHUM, KENDRIC J. NELSON, Dept. of Chemistry, University of Utah, JOEL S. MILLER, Dept. of Chemistry, A.J. EPSTEIN, Deps. of Physics and Chemistry, The Ohio State University — Recently, organic materials both magnetic and non-magnetic have been receiving significant attention for their potential applicability in spintronics devices such as spin-valves, memory devices, spin-transistors etc. Here we report magnetic and X-band FMR studies of an organic based mixed valent Vanadium Hexacyanochromate magnet \(K_{1.54}\text{V}^{\text{III}}\text{V}^{\text{II}}\text{V}^{\text{III}}\text{Cr}^{\text{III}}\text{(CN)}_6\text{(SO}_4\text{)}_{0.16}\text{3.1H}_2\text{O}\) with an ordering temperature well above room temperature (>300K). Temperature dependencies of FMR parameters including intensity, linewidth, resonance field will be discussed in terms of the coexistence of long-range magnetic ordering and spin-glass-like behavior in this material. [1] Øyvind Hatlevik et. al. Adv. Mater. 11, 914 (1999).

12:51PM B27.00007 Origin of edge magnetism in zig-zag graphene nanoribbons , JIEL JUNG, ALLAN MACDONALD, University of Texas at Austin — We explore the physical origins of edge magnetism in zig-zag terminated graphene nanoribbons addressing the role of exchange effects and the band structure in the ferromagnetic alignment of the spins along the edge, the preference of anti-ferromagnetic inter-edge ground state to the ferromagnetic one, and the microscopic physics of the spin stiffness along an edge. Our analysis of the qualitative physics will rest largely on unrestricted Hartree-Fock theory calculations for \(\pi\)-band model Hamiltonian with long-range Coulomb interactions. Unlike Hubbard models, or ab initio LDA calculations, this type of theory can consistently account for non-local exchange effects.

1:03PM B27.00008 Magnetic Properties and Inelastic Neutron Scattering for a Spin Hexamer: Application to the \(V_6\) Molecular Magnets , J. T. HARALDSEN, University of Tennessee, T. BARNES, University of Tennessee/Oak Ridge National Laboratory, J. SINCLAIR, University of Tennessee, J. THOMPSON, University of Tennessee/Oak Ridge National Laboratory, R. SACCI, University of Tennessee, J. TURNER, University of Sussex, UK — We present the study of the magnetic susceptibility and inelastic neutron scattering energies and intensities for a spin hexamer formed by two interacting spin \(S\) and \(S'\) trimers. Using an isotropic Heisenberg Hamiltonian, we conclude that, regardless of spin, the structure factors for the magnetic excitations will have a specific function form which is dependent on the symmetric parts of the hexamer being excited. This work is then compared to previous work performed on two vanadium compounds \((\text{CN})_2\text{H}_2\text{O}_2\text{Na}_2\text{H}_2\text{V}_2\text{O}_7\text{(PO}_4\text{)}_3\text{(OCH}_3\text{)}_2\text{OH}_2\text{O})_2\text{1H}_2\text{O}\) and \(\text{Na}_2\text{H}_2\text{V}_2\text{(SO}_4\text{)}_3\text{(OCH}_3\text{)}_2\text{OH}_2\text{O})_2\text{1H}_2\text{O}\), which are thought to be magnetically well described as trimers of \(S=1/2\) \(V^{4+}\) ions. We show that it is possible to that a very weak inter-trimer interaction exists and we predict the energy and momentum transfer dependence for these compounds that may be observable with inelastic neutron scattering.
Can large magnetic anisotropy and high spin really coexist? ClAUDIA LOOSE, Institute for theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany, ELISEO RUIZ, JORDI CIRERA, JOAN CANO, SANTIAGO ALVAREZ, Departament de Quimica Inorganica and Institut de Recerca de Quimica Teorica i Computacional, Universitat de Barcelona, Diagonal 647,08028, JENS KORTUS, Institute for theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany — This theoretical study discusses the interplay of the magnetic anisotropy and magnetic exchange interaction of two Mn$_{12}$ complexes. Our results for two polynuclear Mn$_{12}$ complexes show a very strong dependence of the D value on the spin of the ground state while the energy barriers are practically constant. Thus, complex 2 with a large spin (S = 12) favoured by ferromagnetic interactions has a small D value, while the lower spin complex 1 (S = 4) has a large D value. Therefore we suggest, that a large magnetic anisotropy is not favoured by a high spin state of the ground state.


1:51PM B27.00009 Time Evolution of Electric Properties of Mn$_{12}$-Acetate Film Measured with Self-assembled Tunneling Junction, LIANXI MA, Dept. of Physics, Texas A&M University, CHI CHEN, GLENN AGNOLET, Texas A&M University — we report the results of tunneling measurement of Mn$_{12}$-Ac thin film (~2 monolayer) at the time right after the film is made and after 6 months. We found that for the fresh film the differential conductance can change suddenly at bias voltage about -0.1 V and staircase form of $I$ − $V$ curves are observed. At about 0 V bias voltage, we see the conductance changes from minimum to maximum as the initial resistance decreases. For the film stored for 6 months, however, all of these properties have been lost and high frequency oscillation on conductance is frequently observed. Also for the stored sample, clean $I$ − $V$ curves are rarely seen. All of these results indicate that deterioration of the molecules after 6 months.

2:03PM B27.00013 Order from disorder in the molecular-based spin ladder Cu(Qnx)Br$_2$, CHRISTOPHER LANDEE, CHRIS SATALINE, BRIAN KEITH, IGOR PARTOLA, MARK TURNBULL, Clark University — Copper quinoxaline dibromide is a molecular-based antiferromagnetic spin ladder in which Cu$_2$Br$_4$ dimers are linked into ladders by the quinoxaline molecules. The rung exchange occurs through the bridging bromide ions while the rail exchange occurs through the organic molecules [1]. It is possible to introduce randomness into this ladder by replacing bromide ions by chlorides, by replacing the quinoxaline molecules by the structurally equivalent 2,3-dimethylpyrazine, or by substituting diamagnetic cadmium ions into the copper sites. In all cases, order occurs at low temperatures (4 to 6 K) as evidenced by FC/ZFC studies, hysteresis and remnant magnetizations, as well as sharp anomalies in the susceptibility. [1] C. P. Landee et al, Polyhedron 22, 2325-2329 (2003).

Monday, March 10, 2008 11:15AM - 1:51PM – Session B28 DMP: Focus Session: Optical Properties of Nanostructures II: Graphene, Graphite and Related Materials Morial Convention Center 220

11:15AM B28.00001 Optical studies of multilayer graphene in magnetic fields, HSIANG-LIN LIU, Department of Physics, National Taiwan Normal University, G. L. CARR, Brookhaven National Laboratory, National Synchrotron Light Source, K. A. WORSLEY, M. E. ITKIS, E. BEKYAROVA, R. C. HADDON, Department of Chemistry, University of California-Riverside, A. N. CARUSO, Center for Nanoscale Science and Engineering, North Dakota State University — We report the optical properties of multilayer graphene thin films grown on silicon substrate. The room-temperature reflectance and transmittance of the samples were measured over the energy range from the far-infrared to near-infrared. To extract the optical constants of the films, we analyzed all of the layers of this thin-film structure using a Drude-Lorentz model. From the parameters obtained, we compute the optical constants. With decreasing temperature, the far-infrared transmittance of the samples is increasing up to 4 % down to 2 K. Interestingly, in an applied magnetic field of up to 10 Tesla, the giant positive magneto-optical effects over 20 % are observed in the far-infrared region from 2 K to 300 K. Possible origin of these will be discussed.

Research at the NSLS is supported by the Department of Energy under contract DE-AC02-98CH10886
11:27AM B28.00002 Edge states and optical transition energies in carbon nanoribbons\(^1\) JIE JIANG, WENCHANG LU, JERRY BERNHOLC, Center for High Performance Simulation and Department of Physics, North Carolina State University, Raleigh, NC 27695-7518 — The local density of states (LDOS) of edge states and optical transition energies in carbon nanoribbons are investigated with density-functional calculations. The LDOS in either magnetic or non-magnetic phases show peaks both below and above the Fermi level. The peaks in the two phases are localized in different energy ranges. Moreover, the LDOS in the two phases have the same decay shapes. The defects at zigzag edges are found to destroy spin-polarization in edge states. They also tend to increase the decay length in edge states by mixing defect and edge states. Thus, the LDOS measured by scanning tunneling spectroscopy shows different features depending on the edge quality. We also find that the optical transition energies \( E_{\text{opt}} \) are not affected by the spin-polarization. However, edge effects tend to increase \( E_{\text{opt}} \) values by 1.25/W, where \( W \) is the ribbon width. Therefore, the ratios of \( E_{\text{opt}} \) in nanoribbons for different \( i \) are changed from those observed in single-wall carbon nanotubes.

\(^1\)We gratefully acknowledge support by DOE, DOD and ONR.

11:39AM B28.00003 Raman Studies of Electron-Phonon Coupling in Graphene and Graphite Intercalated Compounds\(^1\) J. CAMACHO, M. Y. SFEIR, A. T. BOLLINGER, Brookhaven National Laboratory, A. C. WALTERS, C. A. HOWARD, M. ELLERBY, University College London, J. A. MISEWICH, T. VALLA, Brookhaven National Laboratory — Effects of the electron-phonon interaction in carbon-based materials can be seen in many physical properties, ranging from relatively high-Tc superconductivity in doped fullerenes and graphite intercalated compounds to being a limiting factor on the mobility of carriers in carbon nano-tubes. Despite the intensive research, these effects are not completely understood. Here we present Raman scattering studies of several long wavelength optical phonons in different graphite-based materials. We find that the frequency and line-width of some modes are very sensitive to electric field doping and to chemical doping of graphene sheets, reflecting the changes in interactions of these modes with charge carriers in the system.

\(^1\)This work was supported by the DOE under contract number DE- AC02-98CH10886.

11:51AM B28.00004 Optical Selection Rule from Inversion Symmetry Breaking and Valley Optoelectronics in Graphene, WANG YAO, DI XIAO, QIAN NIU, The University of Texas at Austin — Inversion symmetry breaking allows contrasted circular dichroism in different \( k \)-space regions, which takes the extreme form of optical selection rules for interband transitions at high symmetry points. In graphene systems with broken inversion symmetry, this enables valley dependent interplay of electrons with light of different circular polarizations, in analogy to spin dependent optical activities in semiconductors. We discuss graphene based valley optoelectronics applications where light polarization information can be interconverted with electronic information.

12:03PM B28.00005 Gate-Variable Optical Transitions in Graphene, FENG WANG, UC Berkeley, YUANBO ZHANG, CHUANSHAN TIAN, CAGLAR GIRIT, ALEX ZETTL, MICHAEL CROMMIE, Y. RON SHEN — Two-dimensional graphene monolayers and bilayers exhibit fascinating electrical transport behaviors. Using infrared spectroscopy we find that they also have strong interband transitions and, remarkably, their optical transitions can be significantly modified through electrical gating. This unique gate-dependence of interband transitions adds a valuable dimension for optically probing graphene bandstructure. For a graphene monolayer, it yields directly the linear band dispersion of Dirac fermions, while in a bilayer it reveals a dominating van-Hove singularity arising from interlayer coupling.

12:15PM B28.00006 Filling-Factor-Dependent Magnetophonon Resonance in Graphene, KOSTYANTYN KECHEDZHI, Physics Department, Lancaster University, Lancaster, LA1 4YB, UK, MARK GOERBIG, JEAN-NOEL FUCHS, Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS UMR 8502, F-91405 Orsay, France, VLADIMIR FALKO, Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK — We describe a peculiar fine structure acquired by the in-plane optical phonon at the \( \Gamma \)-point in graphene when it is brought into resonance with one of the inter-Landau-level transitions in the material. The effect is most pronounced when this lattice mode is in resonance with inter-Landau-level transitions \( \nu \equiv 0 - \nu_0 \equiv 1 \) at a magnetic field \( B_0 \approx 30 \) T. The predicted mode splitting may be used to measure directly the strength of the electron-phonon coupling, and also to distinguish between circularly (left- and right-hand) polarized lattice modes. A similar effect is predicted in bilayer graphene in lower magnetic fields.

12:27PM B28.00007 Raman Spectrum of Strained Single Layer Graphene\(^1\), MINSHENG WANG, SONG HAN, KANG L. WANG, UCLA — Two-dimensional single layer graphene (SLG) films are very attractive due to their unique electrical and optical properties. In this work, silicon nitride, silicon oxide and polyimide are used to induce strain in SLG sheets. Micro-Raman spectra reveal the evolution of graphene feature peaks under various stress conditions. Different peak position, width and shape are observed due to different stress type, level and direction. Changes of the second order D peaks show that strain affects not only the phonon spectrum but also the electron band through a double resonant Raman process. Relative intensity changes between D and G bands indicate that defects are introduced into graphene during some of the deposition processes, which usually are not observed in spin-coated SLG samples. Strain effects also can be utilized to further modify the electron band structure of graphene.

\(^1\)This work was in part supported by FCRP-FENA (Functional Engineered Nano Architectures).

12:39PM B28.00008 Infrared probe of charge dynamics in graphene transistors, ZHIQIANG LI, University of California, San Diego, ERIK HENRIKSEN, Columbia University, ZHIGANG JIANG, Columbia University/NHMFL, ZHAO HAO, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, PHILIP KIM, Columbia University, HORST STORMER, Columbia University/Bell Labs, DIMITRI BASOV, University of California, San Diego — We report on infrared (IR) spectroscopy of charge dynamics in monolayer graphene. IR reflectance and transmission measurements were performed on graphene transistors as a function of gate voltage. From these data, we obtained the optical conductivity of graphene at various carrier densities. The dominant feature of the optical conductivity is an interband transition with the onset at twice the Fermi energy, which evolves systematically with gate voltage. Similar behavior was observed with the Fermi level on either side of the Dirac point. We will compare these results with theoretical predictions and discuss several new aspects of the charge dynamics in graphene uncovered by this work.

12:51PM B28.00009 The G-band phonon frequency in single layer graphene, HYUNGBIN SON, ALFONSO REINA, MILDRED DRESSELHAUS, JING KONG, Massachusetts Institute of Technology — Recent experimental studies on the high-frequency phonon modes of as-deposited \( n \)-graphene layer (nGL) films report that the frequency of the G-band in single graphene layer is generally higher than that in nGL films (n\( \equiv 2 \)) and highly ordered pyrolytic graphite (HOPG). However, our results show that the frequency of the G-band in single graphene layer approaches that in HOPG when the single graphene layer transferred to different substrate, sonicated, or exposed to \( \text{NaOH} \). These results suggest that the difference in the frequency of the G-band in single graphene layer and HOPG is due to the strain generated in the deposition process.
1:03PM B28.00010 Spatially resolved and polarized Raman spectroscopy of graphene. 
DUHEE YOO, HYERIM MOON, HYEONSOOK CHEONG, Sogang University — Graphene samples were prepared by micromechanical cleavage of graphite flakes on silicon wafer, which was covered with a 300-nm silicon oxide layer. Raman spectra of a single-layer graphene were clearly differentiated from those of a few layers of graphene sheets. We compared the spatially resolved micro-Raman spectra with atomic force microscopy to determine the number of layers for each sample, and variations of Raman spectra, which intensity and shift of Raman peak, were observed through the Raman image. The Raman G peak, corresponding to Raman active mode \(E_2g\), was observed at \(\sim -1590\) cm\(^{-1}\), and \(G^*\) peak due to double resonance Raman scattering was observed at \(\sim -2700\) cm\(^{-1}\). We performed polarized Raman spectroscopy of a single-layer graphene. The intensity of G peak was independent of polarization, in agreement with Raman tensor calculation. The variation of Raman intensity of \(G^*\) peak was measured as a function of the analyzer angle. The intensity was maximum for parallel polarization and was minimum for perpendicular polarization. The depolarization ratio was 1/3.

1:15PM B28.00011 Probing Edge defects in \(n = 1, 2, \ldots\) Graphene Layer system via Raman Scattering. 
HUMBERTO GUTIERREZ, AWNISH GUPTA, PETER EKLUND, Pennsylvania State University — Results of a micro-Raman study (spot size \(\sim 0.7\) microns; 514.5 nm excitation) of an edge (or boundary) of \(n\)-layer graphene films is presented. Graphene \((n=1\text{ layer})\) exhibits a very narrow Lorentzian D-band at \(\sim 1344\) cm\(^{-1}\) with FWHM \(\sim 15\) cm\(^{-1}\). For \(2<n<5\), this narrow peak is found to split into four bands. Interestingly, the D band intensity of the edge is quite strong (1/4 of the G-band). If the defects are truly localized on the edge, this implies a better resonance than found for defects at the interior, or, on the other hand, the range of the defects may extend a long distance into the interior of the films and involve many sites. Polarized Raman studies on this D band were made with the incident field at an angle \(\theta\) with respect to the average direction of the edge. The scattered light was collected either parallel (H) or perpendicular (V) to the edge. The polar intensity plots \(I_H(\theta)\) and \(I_V(\theta)\) were found to exhibit a quadrupolar and dipolar pattern, respectively.

1:27PM B28.00012 X-ray absorption spectroscopy of graphite oxides. 
HAE-KYUNG JEONG, BK21 Physics Division, Center for Nanotubes and Nanostructured Composites, Sungkyunkwan University; LEYLA COLAKEROL, Department of Physics, Boston University, Boston, MA 02215, USA; HAN-JIN NOH, Department of Physics, Chonnam National University, Gwangju 500-757, Korea; YUN PYO LEE, MEI HUA JIN, BK21 Physics Division, Center for Nanotubes and Nanostructured Composites, Sungkyunkwan University, PER-ANDERS GLANS, Department of Physics, Boston University, Boston, MA 02215, USA, JAE-YOUNG KIM, Pohang Accelerator Laboratory & Department of Physics, POSTECH, KEVIN E. SMITH, Department of Physics, Boston University, Boston, MA 02215, USA, CHONG YUN PARK, YOUNG HEE LEE, BK21 Physics Division, Center for Nanotubes and Nanostructured Composites, Sungkyunkwan University — We have investigated electronic structures of graphite oxide using x-ray absorption spectroscopy, and variations of Raman spectra, which intensity and shift of Raman peak, were observed through the Raman image. The polar intensity plots \(I_H(\theta)\) and \(I_V(\theta)\) were found to exhibit a quadrupolar and dipolar pattern, respectively.

1:39PM B28.00013 Symmetry breaking in epitaxial graphene probed by ARPES. 
AARON BOSTWICK, TAISUKE OHTA, JESSICA MCCHESNEY, Lawrence Berkeley National Lab, K. V. EMTSEV, TH. SEYLLER, University of Erlangen, KARSTEN HORN, Fritz Haber Institute, ELI ROTENBERG, Lawrence Berkeley National Lab — The energy bands of n-doped graphene on SiC(0001) have been observed to deviate significantly from the expected conical shape near the Dirac crossing[Bostwick et al 2007, Zhou et al 2007]. Two scenarios have been proposed to explain these deviations, either as originated from the real part of the electronic self-energy due to many-body interactions[Bostwick et al], or from “A–B” symmetry-breaking due to chemical interactions between the graphene and the underlying layer[Zhou et al]. In this talk we present a number of arguments against the A–B symmetry breaking scenario, among which is the observed k-dependent intensity of the Fermi surface as measured by ARPES. We show that the observed intensity distribution is directly sensitive to the degree of A–B symmetry breaking and show that the upper limit for an energy gap in graphene on SiC is much smaller than the observed deviations in the band structure.


11:15AM B29.00001 Intrinsic and Extrinsic Limits of Mobility in Graphene. 
MICHAEL S. FUHRER, Department of Physics and Center for Nanophysics and Advanced Materials, University of Maryland — Graphene is an exciting new condensed matter system, both for the opportunity to observe the physics associated with massless Dirac Fermions in the laboratory, and because of materials parameters which make it attractive for technological applications. However, in the few years since the experimental realization of graphene, progress toward cleaner (higher mobility) samples has largely stalled. I will discuss experiments performed on atomically-clean graphene on SiO\(_2\)[1] in ultra-high vacuum to determine the intrinsic and extrinsic limits of mobility in graphene[2,3], which point out both the promise of the material as well as the technological challenges that lie ahead in realizing better graphene samples. Intrinsic scattering by the acoustic phonons of graphene[3] limits the room-temperature mobility to \(2 \times 10^5\) cm\(^2\)V\(\cdot\)s\(^{-1}\) at a carrier density of 10\(^{12}\) cm\(^{-2}\), higher than any known material. However, extrinsic scattering due to charges in the substrate[2] and substrate polar optical phonons[3] currently impose much more severe limits on the mobility, pointing out the importance of substrate choice for graphene devices[4].

1 Supported by U.S. ONR grant N000140610882 and U.S. NSF grants CCF-06-34321 and DMR-05-20471.
12:03PM B29.00003 Single-particle relaxation time versus scattering time in 2D graphene layers

EUYHEON HWANG, SANKAR DAS SARMA, University of Maryland, College Park — We calculate the transport scattering time ($\tau_s$) and the single particle relaxation time ($\tau_r$) for disordered graphene in the lowest order of the electron-impurity interaction (Born approximation). We find that the ratio of $\tau_r$ to $\tau_s$ is always greater (less) than two for charged Coulomb (short-ranged neutral) scatterers. Thus, the calculated scattering time ratio can be a good criterion of directly selecting the dominating scattering mechanism in graphene. As a direct consequence of the simple form of our results we calculate graphene mobility, damping rate, and density of states of single particle state.

1This work was supported by U.S. ONR, LPS-NSA, and SWAN-NSF-NRI.

12:15PM B29.00004 The Coulomb Impurity Problem in Graphene

VITOR PEREIRA, JOHAN NILSSON, ANTONIO CASTO NETO, Boston University — We address the problem of an unscreened Coulomb charge in graphene and calculate the local density of states and displaced charge as a function of energy and distance from the impurity. This is done nonperturbatively in two different ways: (1) solving the problem exactly by studying numerically the tight-binding model on the lattice and (2) using the continuum description in terms of the 2D Dirac equation. We show that the Dirac equation, when properly regularized, provides a qualitative and quantitative low energy description of the problem. The lattice solution shows extra features that cannot be described by the Dirac equation: namely, bound state formation and strong renormalization of the van Hove singularities.


12:27PM B29.00005 Coulomb Impurity Screening in Graphene

VALERI KOTOV, Boston University — I will discuss the vacuum polarization charge density around a Coulomb impurity with charge $Ze$. Perturbation theory in powers of $Ze$ is the effective coupling constant in graphene), shows that the polarization charge is localized at the impurity site. An exact calculation, based on the Green’s function in a Coulomb field, leads to a non-perturbative result, valid to all orders in $Ze$ [1]. Taking into account also electron-electron interactions in the Hartree approximation, we solve the problem self-consistently in the subcritical regime, where the impurity has an effective charge $Z_{\text{eff}}$, determined by the localized induced charge. We find that an impurity with bare charge $Z = 1$ remains subcritical, $Z_{\text{eff}} < 1/2$, for any $\alpha$, while impurities with $Z = 2, 3$ and higher can become supercritical at certain values of $\alpha$.


LUIS BREY, ICMM-CSIC (Spain), HERBERT FERTIG, Indiana University — In this work we present a detailed study of the conductive properties of wide graphene strips, with two different models for the source and drain leads. We reconfirmed that for undoped graphene, the system can be described by a conductivity in the $L \rightarrow \infty$ limit even when defects are absent from the system, and examined this behavior with respect to a broad range of lead parameters. Our results indicate that the conductance is relatively insensitive to the electronic structure of the leads. We then compute the conductivity of a simple three stripe spin-valve device with graphene acting as the non-magnetic material between the ferromagnetic leads. Two types of ferromagnetic lead systems were considered: one with a single ($s$) orbital for each spin state, with band centers separated in energy to induce spin polarization, and another with a narrow d band which was taken to be spin-polarized. We find that the conductivity depends only weakly on the relative spin orientations of the leads, and therefore the magnetoresistance is rather small for most circumstances, largely due to the insensitivity of the conductivity with respect to conditions in the leads. Our results indicate that, although graphene has properties that make it attractive for spintronic devices, the performance of a graphene-based spin-valve is likely to be poor.

12:51PM B29.00007 Spin transport in graphene strongly coupled to ferromagnetic leads

JELENA TRBOVIC, HAGEN AURICH, GUNNAR GUNNARSSON, CHRISTIAN SCHONENBERGER, University of Basel — We study low temperature spin transport in graphene layers by using NiPd alloy as ferromagnetic contacts. This type of contacts has been successfully used in realizing carbon nanotube-based spin devices. The measurements are done in the temperature range between 240 mK and 1.6 K with average electrode separation of 0.7 µm. We find a clear two-terminal spin-valve signal while sweeping the magnetic field in plane of the device, with about 3% effect. However, the signal rapidly decays with increasing temperature and vanishes above 1.6 K. We believe that the observed rapid dephasing is due to the strong coupling of PdNi contacts to the graphene layer. In addition, three-terminal measurements (quasi non-local) have been done in the same temperature range in order to study the influence of a single NiPd electrode on the observed spin transport.

1This work has been supported by the Swiss Institute on Nanoscience, the Swiss National Science Foundation and the EU HYSWITCH project.

1:03PM B29.00008 Interference of Electron Waves in a Ballistic Graphene Transistor

SUNGJAE CHO, MICHAEL FUHRER — We have prepared single- and few-layer graphene samples by mechanical exfoliation of Kish graphite on SiO$_2$/Si substrates. We have fabricated graphene field-effect transistors by electron beam lithography followed by thermal evaporation of Cr/Au or Permalign source and drain electrodes; the conducting silicon underneath 300 nm silicon dioxide serves as a back gate electrode. We find that at low temperatures that the two-dimensional plot of conductance as a function of gate voltage and drain voltage shows an interference pattern of maxima and minima which occur along diagonal lines. We analyze the pattern in terms of interference of electron waves reflected between source and drain electrodes. The slope of the lines measures the compressibility of the two-dimensional electron system, and has strikingly different dependence on carrier density (gate voltage) for single- and few-layer graphene samples, as expected theoretically.

1Interference of Electron Waves in a Ballistic Graphene Transistor
1:15PM B29.00009 Local Gating of Graphene Devices via Contactless Top Gates, JAIRO VELASCO JR., GANG LIU, CHUN NING LAU, Department of Physics and Astronomy, University of California at Riverside — Graphene devices with local electrostatic gates are promising candidates for investigation of novel phenomena such as Klein tunneling and the veselago lensing effect. However, it is experimentally challenging to fabricate local gates without inadvertent introduction of dopants or defects. We have developed a novel lithography process that enables fabrication of contactless, suspended top gates above single and bi-layer graphene devices. Using this technique, we have demonstrated graphene p-n junctions. We will discuss latest progress towards electrical transport of such devices in the zero-magnetic field regime, as well as in the quantum Hall regime.

1:27PM B29.00010 Current-Voltage Characteristics of Electrolyte-Gated Graphene Field-Effect Transistors$^1$, INANC MERIC, SEBASTIAN SORGENFREI, MELINDA HAN, BARBAROS OZEYILMAZ, PHILIP KIM, KENNETH SHEPARD, Columbia University — We investigate the current-voltage characteristics of graphene field-effect transistors (FET) with ionic-solution gating. Single-layer graphene FETs are fabricated with different device dimensions and electrolytically gated with a potentialistat in which a Pt counter electrode and an Ag/AgCl reference electrode in a feedback configuration hold the solution at a desired potential. This setup enables the gating of graphene with high efficiency due to the short Debye length and high dielectric constant in ionic solutions, leading to enhanced measured transconductances. Electrolytic gating has direct applicability to field-effect sensor applications of graphene devices.

$^1$This work is supported in part by the SRC Focus Center Research Program through the C2S2 Center.

1:39PM B29.00011 Fabrication of gated suspended graphene devices, KIRILL BOLOTIN, MARTIN KLIMA, KENNETH SIKES, GEOFF FUDENBERG, JAMES HONE, PHILIP KIM, HORST STORMER, Columbia University — We find that graphene acts as a catalyst for the vapor-phase etch of silicon dioxide: silicon dioxide under graphene is etched much faster compared to the bare surface. This is consistent with the presence of a trapped water layer between graphene and the silicon dioxide substrate which accelerates etching of the substrate. This unusual property allows us to fabricate devices where a large-area graphene flake is suspended over a micron-sized trench with the unetched silicon substrate serving as a gate electrode. Electronic transport in the resulting devices suggests enhanced sample mobilities near the Dirac point.

1:51PM B29.00012 High resolution, temperature dependent Raman spectroscopy of graphene, SEBASTIAN RÉMI, CONSTANZE METZGER, BILLY HUBBARD, CLAIRE THOMAS, BENNETT B. GOLDBERG, Boston University, Department of Physics, ANNA SWAN, Boston University, ECE — Single and bi-layer graphene are studied with high resolution, temperature dependent Raman scattering. The electron-phonon coupling in graphene depends sensitively on both the concentration of charge carriers and the temperature. Raman spectroscopy directly probes electron-phonon coupling, and has been used to examine the stiffening of the G-band, phonon damping [1] and spatial inhomogeneities in the carrier density [2]. Our measurements are performed between room temperature and 4K in a confocal scanning Raman system. The samples are back-gated, allowing us to tune the carrier density and spectroscopically map the Raman response. We will discuss our recent measurements. [1] J. Yan, Y. Zhang, P. Kim, and A. Pinczuk, Phys. Rev. Lett. 98, 166802 (2007) [2] C. Stampfer, et al. Arxiv, cond-mat 0709.4156v1.

2:03PM B29.00013 Studies of limitations on the mobility and mean free paths in graphene devices.$^1$, XU DU, IVAN SKACHKO, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — The Dirac Fermion nature of the quasiparticles in graphene has led to many predictions for novel phenomena such as specular Andreev reflections at graphene-superconductor interfaces and a negative index of refraction for transmission of charge across graphene p-n junctions. These predictions presuppose ballistic transport, which requires long mean free paths compared to the distance between leads. However, within current fabrication techniques, the mean free paths of charge carriers in graphene devices are often too short for ballistic transport. The reduced mean free path is primarily due to excess scattering introduced by extrinsic factors such as material imperfections, substrate contamination, e-beam resist residue, chemical doping, contact potential and contact geometry. We will discuss the results of systematic studies of extrinsic factors, highlighting the case of graphene SNS weak links, and will propose strategies to increase the mean free path.

$^1$Work supported by DOE DE-FG02-99ER45742, NSF-DMR-0456473 and ICAM.

Monday, March 10, 2008 11:15AM - 2:15PM
Session B30 DMP: Focus Session: Carbon Nanotubes and Related Materials III: Synthesis
Morial Convention Center 222

11:15AM B30.00001 Novel Functions in Double Walled Carbon Nanotubes, MORINOBU ENDO, Shinsu University — Nano-sized carbon nanotubes with hollow core were observed when hydrocarbons were catalytically decomposed in the existence of nano-sized catalyst such as iron at higher temperature. Up to now, this catalytic chemical vapor deposition (CCVD) method has been utilized as the most powerful technique for the selective and large-scale production of carbon nanotubes. Since large amount of multi-walled carbon nanotubes (up to 250 ton/year) are available, much efforts has intensified on the development of their industrial usages. A recent hot topic has focused on the synthesis of double walled carbon nanotubes (DWNTs) because these tubes are more thermally and chemically stable when compared to single wall carbon nanotubes (SWNTs); they also exhibiting the 1D character of a quantum wire. In addition, DWNTs could also be used in the fabrication of electron field emitter and nano-composites. Very recently, we have successfully prepared highly pure and crystalline DWNTs by the combination of the CCVD and the subsequent oxidative purification process. In this talk, I will describe the preferential growth of DWNTs over SWNT or MWNTs, their structural characterizations using variuos analytis techniques and their possible applications. We found that these coaxial tubes consist of two relatively round, small and homogeneous-sized (below 2 nm in the outer shell) concentric tubes and are packed in a hexagonal array. Then, I will discuss a novel and stable structure consisting of flattened tubes consisting two SchwNTs via the coalescence of two adjacent tubes, chemical doping effect as a tunable way of electronic structure of DWNTs, and formation of atomic scale metal wires in the hollow core of DWNTs. Finally, I will report their transport properties as well as their performance in field effect transistors as compared with those of SWNTs. Therefore, in the near future, it may be possible that DWNTs replace SWNTs in specific carbon nanotube devices used today.

11:51AM B30.00002 Electron Spin Resonance in Single-Walled Carbon Nanotubes$^1$, W. D. RICE, J. KONO, Rice University — We have performed electron spin resonance (ESR) measurements on various types of single-walled carbon nanotube (SWNT) samples. As catalyst particles were chemically removed from the SWNTs, the linewidth of the conduction electron spin resonance (CESR) signal became smaller, reaching 43 G at 5 K for acid-purified HiPco SWNTs. For every type of SWNT tested, a ferromagnetic resonance (FMR) signal was observed; we show that this is attributed to catalyst particles. The g-factor for the CESR signal was slightly shifted from the free electron value; as purity increased, the resonance moved closer to $g = 2.003$. The conduction electron signal increased as the temperature was decreased, indicating that we are observing both Pauli and Curie paramagnetism. No spin gap for either laser-oven acid-purified or HiPco acid-purified SWNTs was seen when the temperature was taken from 295 K to 5 K. In addition, the FMR signal decreased as the temperature was decreased. SWNTs suspended in aqueous surfactant solutions were also measured. As a function of purity, the FMR signal was substantially decreased. We show that as a function of metal catalyst content, the ESR lineshape of SWNTs changes significantly.

$^1$This work was supported by ARO Grant No. 49735-PH.
12:03PM B30.00003 IPS verification of the integrity of CNTs walls after purification. PATRICIO HABERLE, SAMUEL HEVIA, RODRIGO SEGURA, UTFSM, MANISH CHHOWALLA, Rutgers University — We report results from measurements by inverse photoemission spectroscopy (IPS) from single wall carbon nanotubes (SWCNTs). We have used this technique to verify the influence of strong purification procedures on the integrity of the tube walls. The purification included an HNO$_3$ immersion in a solution for 3 hours, before a 400 °C annealing. Even though the thin layers of CNTs present a high conductivity, the treated tubes trap the electronic charges from the IPS electron beam. A possible explanation for this apparent inconsistency is that the acid treatment induces the formation of charge traps in the outside tubes of the bundles. RAMAN spectroscopy from the same samples, with and without the acid treatment, show almost no variations. The IPS signal is extremely sensitive to the conditions of the tube’s external wall, while Raman spectroscopy can detect signals from inner tubes. Using IPS may then prove useful to determine electronic quality of CNTs arrays.


12:27PM B30.00005 Controlled Fabrication of Single Electron Transistors from Single-Walled Carbon Nanotubes. PAUL STOKES, SAIFUL I. KHONDAKER, NANOSCIENCE TECHNOLOGY CENTER AND DEPARTMENT OF PHYSICS, UNIVERSITY OF CENTRAL FLORIDA TEAM — Single-walled carbon nanotubes (SWNTs) are considered to be an ideal material for quantum electronic applications such as single electron transistors (SETs). However, fabrication of SET based devices is still in its infancy. Controlled fabrication of SWNT-SETs has been demonstrated by introducing kinks using AFM. However, AFM manipulation is time consuming and reproducibility can be extremely challenging. Here, we show a novel approach to fabricate controllable and reproducible SETs using SWNT. SWNTs were placed on 100 nm wide local Al/Al$_2$O$_3$ bottom gates and then contacted with Pd source and drain electrodes with 1 um spacing on Si/SiO$_2$ substrates. The Al gate serves two purposes: (i) it defines tunnel barriers at the edges of the gate electrodes by introducing buckles, and (ii) it acts as a local gate to tune the number of carriers in the central island. Low temperature electronic transport measurements show coulomb oscillations up to 125 K. The stability diagram shows a charging energy of $\sim 13$ meV and energy level spacing of $\sim 5$ meV. These energies are consistent with a quantum dot size of $\sim 100$ nm, thus verifying the dot is defined and controlled by the 100 nm wide aluminum oxide gate.


12:51PM B30.00007 Structural and Electronic Properties of Single-Walled Carbon Nanotube Heterojunctions$^1$. JOYDEEP BHATTACHARJEE, Molecular Foundry, LBNL., YOUNG WOO SON, Dept. of Physics, Konkuk Univ., Seoul, Korea., BHUPESH CHANDRA, JAMES HONE, Dept. of Mech. Eng., Columbia Univ., JEFFREY B. NEATON, Molecular Foundry, LBNL. — Inspired by recent experiments$^1$, we present a systematic approach to construct structural models of mostly linear single walled carbon nanotube (SWCNT) heterojunctions. A minimum number of 5-7 defects is found to be required to join two SWCNTs of differing chiralities. Using nearest-neighbor tight-binding and first-principles density functional theory, we explore the sensitivity of the heterojunction electronic structure and transport properties to different arrangements of the interfacial 5-7 defects, and discuss their implications for future experiments and nanoelectronic applications.

References


1:03PM B30.00008 Synthesis and Structure of Carbon Nanotube Junctions and Co$_8$S$_8$ Nanowire-filled Carbon Nanotubes$^1$. WENZHI LI, GAOHUI DU, Florida International University, NANOPHYSICS TEAM — We describe the synthesis of carbon nanotube junctions and Co$_8$S$_8$ nanowire-filled carbon nanotubes by pyrolysis of thiophene on cobalt catalyst in chemical vapor decomposition. The formation of these nanostructures is strongly dependent on the thiophene vapor concentration during the material synthesis. The carbon nanotube junctions have hollow channels while the filled carbon nanotubes have solid Co$_8$S$_8$ cores. The encapsulated Co$_8$S$_8$ nanowires are single crystals, and their lengths are about 10 $\mu$m with their [110] direction parallel to the axis of the carbon nanotubes. It is postulated that the filling of the Co$_8$S$_8$ nanowires results from the volume increase of the catalyst induced by a phase transition from cobalt to cobalt sulfide and the spatial confinement of the carbon nanotubes as nano-molds.

$^1$This work was supported by the NSF Grant No. DMR-0548061.
1:15PM B30.00009 Adsorption of Alcohols and Alkanes on Single-Walled Carbon Nanotubes  

ERIK ALLDRIDGE, STEFAN BADESCU, THOMAS REINECKE, NADEEP BAJWA, F. KEITH PERKINS, ERIC SNOW, Naval Research Laboratory  
Recent experiments with arrays of carbon nanotubes (CNTs) reveal a strong electrical response during exposure to polar alkane derivatives such as linear alcohols \( C_nH_{2n+1}OH \), which is in contrast with the weak response to linear alkanes \( C_nH_{2n+2} \). To develop an understanding of the microscopic mechanisms involved, we perform detailed \textit{ab initio} calculations of adsorption geometries and charge configurations for the size parameter \( n \) from 1 to 8 on pristine zig-zag and armchair CNTs. We use Density Functional Theory with localized orbitals in a cluster approach, along with the Möller-Plesset functional appropriate for the weak interactions of physisorption for these systems. We find that adsorption energies are larger for alcohols than for alkanes and increase linearly in energy with length of the molecule \( n \) for both alcohols and alkanes (at 35 meV and 40 meV per additional \( CH_2 \), respectively). This is found to be in good agreement with the binding energy per additional \( CH_2 \) estimated from the fast conductance response measurements for both alcohols and alkanes using a simple kinetic theory model. We estimate small charge transfers for all molecules, which suggest that the electric response is dominated by the scattering from the dipole moments of the adsorbates. [This work is supported by the Office of Naval Research.]

1:27PM B30.00010 Adsorption of neon and tetrafluoromethane on carbon nanohorn aggregates: differences in specific surface area values  

VAIVA KRUNGLEVICIUTE, Southern Illinois University Carbondale, MASAKO YUDASAKA, SUMIO IJIMA, Japan Science and Technology Corporation, c/o NEC Corporation, ALDO MIGONE, Southern Illinois University Carbondale  
We have measured adsorption isotherms for two different adsorbates, neon and tetrafluoromethane, on dahlia-like carbon nanohorn aggregates. The experiments were performed at similar relative temperatures for both gases. The measurements were conducted to explore the effect of adsorbate diameter on the behavior of the resulting adsorbed systems. We measured the effective specific surface area value of the nanohorn sample using both gases, and we found that this quantity was about 22% smaller when we determined this quantity using tetrafluoromethane, the larger molecule. Isothermic heat and binding energy values were also determined from our measurements. We will compare our experimental results with those from a computer simulation study performed by Prof. M. Calib. The simulations help us understand the source of the observed differences in the measured specific surface values, as well as the coverage dependence of the isosteric heat of adsorption for both gases.

1:39PM B30.00011 Application of nanohorns to anti-cancer drug carriers  

MASAKO YUDASAKA, JST, NEC, MINFANG ZHANG, KUMIKO AJIMA, JIN MIYAWAKI, JST, TATSUMI MURAKAMI, KUNIHIRO TSUCHIDA, Fujita Health Univ., SUMIO IJIMA, JST, NEC, Meijo Univ — Potential applications of single-wall carbon nanohorns (SWNH) that have shown no acute toxicity in various tailored animal experiments, to the drug delivery system have been studied. We previously reported that the drugs were able to be incorporated inside SWNH at room temperature through liquid phase, and chemical modifications with hydrophobic molecules enhanced dispersion of SWNHs in aqueous solutions. The modifications with the tumor-targeting molecules were also possible. The contrast agent attachments enabled the in vivo visualization of SWNHs by magnetic resonance imaging. We show in this report how the effects of anti-cancer drugs can be influenced by being incorporated inside SWNHs, and discuss its reasons.

1:51PM B30.00012 Building Physical Carbon Nanoparticles from Small-World Networks: Density Functional Theory Calculations  

JEREMY A. YANCEY, M.A. NOVOTNY, Mississippi State University Dept of Physics and Astronomy, HPCC Center for Computational Sciences, STEVEN R. GWALTNEY, Mississippi State University Dept of Chemistry, HPCC Center for Computational Sciences — We have performed B3LYP/6-31G* Density Functional Theory calculations on carbon cluster nanoparticles built with (pseudo) small-world network topologies to determine whether they are stable and can exist in nature. Such particles may have novel material properties due to their (pseudo) small-world nature [1]. We have embedded a ring of carbons with one or more small-world connections made with and without additional carbon atoms. No carbon is allowed to make more than four bonds. The energy per atom of these (pseudo) small-world carbon systems is compared with benchmark carbon clusters including monocyclic rings, linear rods, graphene fragments, and various fullerences from \( C_{60} \) to \( C_{60} \). The energy per atom and vibrational frequency calculations results for these materials indicate that there are pure-carbon small-world nanomaterials that are reasonable for real world synthesis. We present both NMR and IR spectra for these nanoparticles. [1] M.A. Novotny, et al, J. Appl. Phys, 97, 10B309 (2005).

2:03PM B30.00013 First-Principles Study of Carbon Nanoframeworks Tailored for Hydrogen Storage  

EUNJIA KIM, PHILIPPE WIECK, BALAKRISHNAN NADUVALATH, University of Nevada, Las Vegas, HANSONG CHENG, Air Products and Chemicals, Inc., BORIS YAKOBSON, Rice University — Based on first-principles calculations, we propose a novel class of 3-D materials consisting of small diameter single-walled carbon nanotubes (SWCNTs) functionalized by organic ligands as potential hydrogen storage media. Specifically, we have carried out density functional theory calculations to determine the stable structures and properties of nanoframeworks consisting of \( 5,0 \) and \( 3,3 \) SWCNTs constrained by phenyl spacers. Valence and conduction properties, as well as normal modes, of pristine nanotubes are found to change significantly upon functionalization, in a way that can serve as experimental diagnostics of the successful synthesis of the proposed framework structures. Ab initio molecular dynamics simulations indicate that such systems are thermodynamically stable for on-board hydrogen storage. In order to increase the hydrogen uptake in the interstitial cavity of such nanoframeworks, we are currently investigating the possibility of Li deposition on these nanostructures.

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11:15AM B31.00001 Optical Properties of Free and Embedded Small Nanoparticles  

JUAN IDROBO, Vanderbilt University and Oak Ridge National Laboratory — It is well known that the absorption spectra, as well as the effective dielectric function, of nanoparticles in vacuum or surrounded by a dielectric medium can be obtained by classical Mie and Maxwell-Garnett theories. A limit as to how the particles can be for the theory to apply has not been established. Here I present theoretical results on the optical properties of small Ag, Au, and Si and Ge nanoparticles with tens of atoms in vacuum and in an embedded dielectric medium obtained from first-principles density-functional calculations. In particular, I will discuss the role that d-electron play on the optical properties of Ag and Au nanoparticles, and the cases when classical Mie and Maxwell-Garnett theories can be applied for nanoparticles of just few atoms in size and whose atoms are in bulk-like and not bulk-like positions. Comparison will be made for nanoparticles in vacuum and in an alumina matrix. The quantum-mechanical results indicate that small nanoparticles in alumina can have an imprint on the effective dielectric function that is several times larger than what is expected from Maxwell-Garnett theory for same-size particles. This work was supported by a GOALI NSF grant, DOE, the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, and Alcoa Inc. Collaborators: S. Ögüt, K. Jackson, J. Jellinek, A. Halabica, R. F. Haglund, R. Magruder, S.J. Pennycook and S.T. Panteleides.
The results show previous tight-binding calculations greatly exaggerate the electronic response of large fullerenes. Within linear response theory, the SOS polarizabilities are within 1-3% of the finite-field polarizabilities. The polarizability per carbon atom increases from 1.34 in this series, namely C_{240}, to 4 in C_{2160}. This increase is characterized by determining their static dipole polarizabilities by all-electron density-functional theory. We first determine the dipole polarizabilities of C_{2160} and DE-FG02-06ER46286. Computers and mathematics. The electronic response of C_{2160} and DE-FG02-06ER46286. Computers and mathematics.

The fluctuations in the vibrational free energy depend on the elemental environment which is more pronounced in the case of copper atoms. Correlations between Cu atoms in the Cu-core/Ag-shell structure, with coordination 6 show a bi-modal feature with 2 distinct ranges of bond lengths. A global analysis shows that the d band characteristics with coordination/bond length and environment will also be discussed. In addition, correlations between the fluctuations in the vibrational free energy depend on the elemental environment which is more pronounced in the case of copper atoms.

Overall, our theoretical results exhibit quite good agreement with spectra obtained for Ag clusters trapped in rare-gas matrices. We show that the classical predictions from Mie-Gans theory using the bulk dielectric function of Ag are in rather good agreement with experimental results and TDDFT spectra for the ground state and low-energy isomers of Ag_{n} (n = 10 - 20) are presented. The fluctuation in the vibrational free energy depend on the elemental environment which is more pronounced in the case of copper atoms. Correlations between the d band characteristics with coordination/bond length and environment will also be discussed.

Work was supported in part by NSF-ITR 0428826 and DOE grant DE-FG02-03ER46354.

12:39PM B31.00006 Trends in the Electronic Structure and Vibrational Dynamics of 34 atom Ag-Cu Nanoalloy (Ag_{n}-Cu_{34-n})

1, H. YILDIRIM, A. KARA, T.S. RAHMAN, Department of Physics, University of Central Florida — We report results of a systematic study of the electronic and geometric structures as well as vibrational and thermodynamical properties of Ag_{n}-Cu_{34-n}, using density functional theory and model interaction potentials. A detailed analysis of the effect of coordination and atomic environment shows the limitation of coordination to solely explain the changes in the structural and vibrational characteristics. On the other hand, a combination of coordination and environment, as expressed in the elemental characteristics of the neighbors, shows systematic trends in the bond length and vibrational free energy distribution. In addition, Cu atoms in the Cu-core/Ag-shell structure, with coordination 6 show a bi-modal feature with 2 distinct ranges of bond lengths. A global analysis shows that the fluctuations in the vibrational free energy depend on the elemental environment which is more pronounced in the case of copper atoms. Correlations between the d band characteristics with coordination/bond length and environment will also be discussed.

1Work was supported in part by NSF-ITR 0428826 and DOE grant DE-FG02-03ER46354.

12:03PM B31.00003 Bethe-Salpeter and Quantum Monte Carlo Calculations of the Optical Properties of Carbon Fullerenes

P.R.C. KENT, M.L. TIAVO, F.A. REBOREDO, Oak Ridge National Laboratory, RANDOLPH Q. HOOD, Lawrence Livermore National Laboratory — We have calculated the low energy optical excitations of the carbon fullerenes C_{20}, C_{24}, C_{50}, C_{60}, C_{70}, and C_{80}. Properties are calculated via the GW-Bethe-Salpeter Equation (GW-BSE) and diffusion Quantum Monte Carlo (QMC) methods. We compare these approaches with time-dependent density functional results and with experiment. GW-BSE and QMC have previously shown good agreement for small molecules, but this is the first study of these methods for these larger yet prototypical nanostructures. The first ionization potentials are consistently well reproduced and are similar for all the fullerenes and methods studied. However, electron affinities and first triplet exciton show substantial method and geometry dependence. GW-BSE yields triplet energies around 1 eV below the QMC results. We discuss the possible reasons for these differences. Research at Oak Ridge National Laboratory performed at the Materials Science and Technology Division, sponsored by the Division of Materials Sciences, and at the Center for Nanophase Materials Sciences, sponsored by the Division of Scientific User Facilities, U.S. Department of Energy. Research at Lawrence Livermore National Laboratory was performed under Contract DE-AC52-07NA27344.
**1:03PM B31.00008 Heusler clusters**1. ALEXEY ZAYAK, University of Texas at Austin, SCOTT BECKMAN, Rutgers University, MURILIO TIAGO, Oak Ridge Natl. Laboratory, PETER ENTEL, University of Duisburg-Essen, JAMES CHELIKOWSKY. University of Texas at Austin — Real space pseudopotential calculations are used in order to investigate the properties of Heusler clusters. Bulk-like clusters with various Ni-Mn-Ga compositions have been examined in the size range from 15 up to 169 atoms. Among these compositions the closest to the stoichiometric Ni$_2$MnGa are the most stable. These clusters retain tendency for tetragonal distortion, which is inherited from the bulk properties. Although, the surface effects dominate suppressing the tetragonal structure in the smaller clusters, the bigger clusters develop a bulk-like tetragonal distortion. We predict the existence of switchable Ni-Mn-Ga clusters, which might be of great interest for the nano-Magnetic-Shape-Memory technology.

1This work was supported by the National Science Foundation under Contract No. DMR-0551195, by the U.S. Dept. of Energy under Grants No. DE-FG02-06ER46286 and DE-FG02-06ER15760, by the Computational Material Science Network of the U.S. Dept. of Energy.

**1:15PM B31.00009 Tangential Ligand-Induced Strain in Icosahedral Au13**. LEEROY KRONIK, OLGA GULIAMOV, Weizmann Institute of Science, ANATOLY FRENKEL, Yeshiva University, LAURENT MENARD, RALPH NUZZO, University of Illinois — A quantitative comparison of first principles calculations with extended x-ray absorption fine structure and transmission electron microscopy measurements provides strong evidence that Au$_{13}$ nanocrystals are stabilized in a slightly distorted icosahedral structure by on-top phosphine ligands and a combination of on-top and bridging thiol ligands. Importantly, the ligands change the icosahedral strain (i.e. the radial-tangential bond length ratio) significantly, with the tangential bonds within the Au core exhibiting much more disorder than the radial ones.

**1:27PM B31.00010 Structural Properties and Phase Transitions in Small Gold Nanoclusters**. YANTING WANG, SERGEY RASHKEEV, Idaho National Laboratory — Small gold nanoclusters (below 5 nm in diameter) exhibit good catalytic activity. Molecular dynamics simulations combined with the parallel tempering method have been used to investigate the bulk and surface structural properties and phase behavior of small gold nanoclusters ($10^3$-$10^4$ atoms). For small clusters, the transition from solid to liquid does not occur at a definite temperature. Instead, one gets a temperature range within which the transition state from solid to liquid is observed, and this range become broader for nanoclusters with smaller number of atoms. In this work, we perform an analysis of structural and dynamic properties of gold nanoparticles of different sizes and show that the nature of the solid-liquid phase transition in very small nanoparticles (with tens of atoms) is radically different from that of the mid-sized ones ($10^2$-$10^3$ atoms). The surface characteristics of the particle (the presence of low-coordinated atoms at the surface and the dynamic fluxionality, i.e., an ability of the surface to reconstruct) that define its catalytic behavior are also investigated and analyzed.

**1:39PM B31.00011 The peculiar distribution pattern of Pd on the PdAu bimetallic nanoclusters**1. DINGWANG YUAN, University of California, Irvine, XINGAO GONG, Fudan University, RUQIAN WU, University of California, Irvine — Through systematic density functional calculations, we found that Pd atoms in PdAu nanoclusters may only take the (111) facets while leave the (001) facets with pure Au. This is promoted by the tendency that Pd prefers to form bonds with Au, rather than with Pd. The segregation from the (001) facet to the (111) facet appears to occur easily. The local activity of Pd somewhat depends on the size of cluster and site of substitution. The peculiar distribution pattern of the active constituent should strongly alter the chemical properties of bimetallic nanoclusters toward catalyzing reactions.

1Work was supported by the DOE-BES (grant No: DE-FG02-04ER15611). Calculations are performed on supercomputers in the NERSC.

**1:51PM B31.00012 Computational model for the production of monodisperse silver spheres in solution**1. DANIEL ROBB, IONEL HALACIUGA, VLADIMIR PRIVMAN, DAN GOIA, Clarkson University — We report the results of computational modeling of the production of monodisperse, spherical silver particles through the rapid mixing of reducing agent and silver-amine complex solutions, in the absence of a protective colloid. We find that the process can be modeled effectively by a two-stage reaction mechanism used previously to model the production of gold particles [1]. Here, we treat both the equilibrium concentration of silver atoms and the surface tension of silver particles as free parameters in our simulation, finding that the reaction time scale is fit by a narrow region of this parameter space. As in the previous work on gold particles, a kinetic ‘dimer suppression factor’ is required to limit the number of final particles produced. In addition, we consider an extension of the two-stage reaction model which incorporates the effect of the silver-amine complexation reaction on the availability of Ag monomers. [1] J. Park, V. Privman, and E. Matijevic, J. Phys. Chem. B 105, 11630 (2001).

1This work was supported in part by NSF Grant DMR-0590104.

Monday, March 10, 2008 11:15AM - 2:15PM –
Session B32 GMAG DMP: Focus Session: Nanocontacts and Inhomogeneous Magnetic States

**11:15AM B32.00001 Theory of magnetic interactions and transport in tunnel junctions and point contacts**. EVGENY TSYMBAL, University of Nebraska-Lincoln — No abstract available.

**11:51AM B32.00002 Fabrication of point contacts by FIB patterning**1. B. O’GORMAN, M. TSOI, University of Texas at Austin, Austin, TX — Nanoscale electrical contacts currently receive an increased amount of attention due to their capability to produce extremely high current densities needed, e.g., in experiments on current-driven precession and reversal of magnetization. Here we describe a new technique for the fabrication of such point contacts using a focused ion beam (FIB) patterning. FIB-fabricated point contacts combine the robustness and size-control of other lithographical methods with the flexibility of mechanical techniques to produce contacts to samples of arbitrary shape and composition. After sample coverage with a thin insulating layer (SiO$_2$), an FIB is used to mill a 100-nm-diameter hole through the insulator. Electrical contact to the sample is then made in-situ by filling the hole with a metal (Pt) using the ion beam assisted chemical vapor deposition capability of our FIB system. We have demonstrated the use of two such contacts (as an emitter and collector) in a transverse electron focusing (TEF) experiment. The contacts were made to a single crystal of bismuth, ballistic electrons were injected into the crystal through the emitter, and then focused onto the collector by a magnetic field. We see the expected voltage peaks at the collector as a function of the applied magnetic field.

1This work was supported in part by NSF Grant DMR-06-45377.
12:03PM B32.00003 Electronic excitations in four structurally similar but magnetically different nickel chain compounds. V.C. LONG, Y.H. CHOU, J.A. CROSS, A.C. KOZEN, L.A. LAVOLET, C.A. MILLER-SHELLEY, J.R. MONTAGUE, E.P. PLUMB, Colby College, S.A. MCGILL, X. WEI, National High Magnetic Field Lab, B.R. LANDRY, K.R. MAXCY-PEARSON, M.M. TURNBULL, C.P. LANDEE, Clark University, R.D. WILLET, Washington State University — We report the low temperature zero-field and magnetic-field-dependent optical spectra of four Ni$^{2+}$ chain compounds: NENP (Ni[en]$^2$NO$_2$ClO$_4$), NENB (Ni[en]$^2$NO$_2$BF$_4$), NTNB (Ni[tn]$^2$NO$_2$BF$_4$), and NINO (Ni[tn]$^2$NO$_2$ClO$_4$). The four differ in the counterions isolating the chains and the rings coordinated to the Ni$^{2+}$ ions. Despite the structural similarities, only three of the compounds exhibit the Haldane gap typical of a spin-1 chain; the fourth, NTNB, behaves like spin glass, likely due to finite chain effects. We focus on the near infrared spin-forbidden (SF) electronic $d - d$ transitions and the visible Ni$^{2+}$-to-NO$_2^-$ charge transfer (CT) band. The zero-field absorption spectra differ in the en and tn ring compounds but are nearly identical in compounds with identical rings. The SF and CT band absorption intensities depend on field in a way that reflects the magnetic ground state. In the Haldane compounds, the onset of intensity changes occurs above the crossover field, whereas in NTNB the field-dependent absorption intensities respond to any finite field.

12:15PM B32.00004 Theory and application for chain formation in break junctions. YURIY MOKROUSOV, ALEXANDER THIESS, Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany, STEFAN BLUGEL, Institut fuer Festkoerperforschung, Forschungszentrum Juelich, 52425 Juelich, Germany, STEFAN HEINZE, Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany — We introduce a generic model for chain formation in break junctions by formulating separate criteria for the stability and producibility of suspended monoatomic chains based on total energy arguments. Using first-principles calculations [1], we apply our model to break junctions of 1d and 2d transition-metals (TMs), as well as Ag and Au, including the effects of spin-polarization and spin-orbit coupling. Thereby, we can explain the physical origin of the experimentally observed trend of increasing probability for the creation of long suspended chains in break junctions for 1d-TMs at the end of the series [2] and suppressed chain elongation for 2d elements. Moreover, we clarify why the probability of chain elongation is greatly enhanced by the presence of oxygen in experiments with Au and Ag. Our model also allows us to make predictions on the ballistic transport properties of suspended chains. [1] Y.Mokrousov et al., Phys. Rev. B 72, 045402 (2005). [2] R.H.M.Smit et al., Phys. Rev. Lett. 87, 266102 (2001).

12:27PM B32.00005 Anderson model of local magnetism at a break junction nanocontact. PAOLA GENTILE, SISSA, Democritos, Trieste, Italy, MICHELE FABRIZIO, GIUSEPPE E. SANTORO, EROS TOSATTI, SISSA, Democritos, ICTP, Trieste, Italy — Atoms at break junction nanocontacts in nearly magnetic heavy transition metals such as Pt and Pd may develop a nonzero magnetization. Since here the nanocontact is strongly electronically tied to the two bulk leads, it is not automatically clear what the correct physical picture of the system should be, and in particular whether the nanocontact should or should not become analogous to a Kondo impurity in quantum dot devices. To clarify this, we consider one (or more) impurity sites inserted into a linear chain (representing the nonmagnetic leads), every site endowed with orthogonally degenerate orbitals, large spin orbit coupling, and Hund’s rule exchange; neighboring sites connected by electron hopping and by intersite ferromagnetic exchange. The mean-field solution when the impurity site (where Hund’s rule exchange is made stronger) is locally magnetic shows a ferromagnetic polarization around it, in agreement with realistic density functional calculations for nanocomposites consisting of monatomic chain segments. Our results suggest that this type of nanocontact, regarded as an Anderson impurity, is ferromagnetically coupled to the leads, and hence that Kondo screening does not occur in this case. The physical consequences for the conductance through the chain are discussed.

12:39PM B32.00006 Dynamics of a pinned magnetic vortex. ROBERT COMPTON, University of Minnesota — Disks patterned from soft ferromagnetic films typically form a single magnetic vortex for diameters on the order of a few microns or less. The vortex dynamics include both ordinary spin waves and a gyroscopic mode, in which the vortex core undergoes circular motion about its equilibrium position [1, 2]. This mode has sub-GHz frequencies which ideally depend on the aspect ratio (diameter over thickness) of the disk [2, 3]. We have used time-resolved Kerr microscopy to investigate the gyroscopic mode as a function of the equilibrium position of the core, which can be tuned by an applied field with a sensitivity of ~ 1 nm/Oe. In the limit of high excitation amplitude, the gyrotropic frequency $f_G$ is independent of the vortex core position, as previously predicted and observed [1, 3]. For small amplitudes, however, we observe unexpected fluctuations in $f_G$ as a function of the applied field. The average core displacement between consecutive frequency peaks, as well as the average frequency shift, is observed to be independent of disk diameter. These observations indicate that the fluctuations are due to a distribution of nanoscale defects that pin the vortex core by lowering its energy [4]. Furthermore, they are consistent with a model in which the frequency shift for a particular fluctuation is a direct measure of the interaction energy of the vortex core with one defect. By mapping $f_G$ as a function of orthogonal in-plane static fields, we image the 2D spatial distribution of defects with nanoscale resolution.

1:15PM B32.00007 Angular Dependence of Vortex Annihilation Field in Asymmetric Co Nanodots. RANDY DUMAS, KAI LIU, Physics Department, UC Davis, THOMAS GREDIG, CHANG-PENG LI, IVAN K. SCHULLER, Physics Department, UC San Diego — Magnetization reversal via a vortex state is a common occurrence in sub-micron magnetic nanodots. We have investigated arrays of 500 nm polycrystalline Co dots prepared by e-beam lithography. The circular symmetry of the dots has been broken by introducing a flat edge to the dots. Magneto-optical Kerr effect (MOKE) measurements and micromagnetic simulations confirm the reversal mechanism of the dots is via the nucleation, propagation, and annihilation of a vortex core. The asymmetric dot shape favors vortex nucleation from the flat edge and therefore allows for control over the vortex chirality. Additionally, by modifying the applied field sweep, we can control which side of the dot the vortex annihilates from. We have studied the vortex annihilation field as a function of the angle between the applied field and the flat edge of the dot. At small angles, the annihilation field depends on the chirality of the vortex and annihilation is easier from the flat edge of the dot. The difference in annihilation fields for the two chiralities is strongly dependent on the angle of the applied magnetic field. This behavior is due to the complex motion of the vortex core across an asymmetric dot during reversal. This work supported by ACS-PRF, AFOSR-MURI, and the Alfred P. Sloan Foundation.


$^1$This work was done in collaboration with Te-Yu Chen and Paul A. Crowell and was supported by NSF DMR04-06029 and the NSF NNIN Program.

Author’s present address: National Institute of Standards and Technology, Gaithersburg, MD.

1:15PM B32.00007 Angular Dependence of Vortex Annihilation Field in Asymmetric Co Nanodots. RANDY DUMAS, KAI LIU, Physics Department, UC Davis, THOMAS GREDIG, CHANG-PENG LI, IVAN K. SCHULLER, Physics Department, UC San Diego — Magnetization reversal via a vortex state is a common occurrence in sub-micron magnetic nanodots. We have investigated arrays of 500 nm polycrystalline Co dots prepared by e-beam lithography. The circular symmetry of the dots has been broken by introducing a flat edge to the dots. Magneto-optical Kerr effect (MOKE) measurements and micromagnetic simulations confirm the reversal mechanism of the dots is via the nucleation, propagation, and annihilation of a vortex core. The asymmetric dot shape favors vortex nucleation from the flat edge and therefore allows for control over the vortex chirality. Additionally, by modifying the applied field sweep, we can control which side of the dot the vortex annihilates from. We have studied the vortex annihilation field as a function of the angle between the applied field and the flat edge of the dot. At small angles, the annihilation field depends on the chirality of the vortex and annihilation is easier from the flat edge of the dot. The difference in annihilation fields for the two chiralities is strongly dependent on the angle of the applied magnetic field. This behavior is due to the complex motion of the vortex core across an asymmetric dot during reversal. This work supported by ACS-PRF, AFOSR-MURI, and the Alfred P. Sloan Foundation.
1:27PM B32.00008 Influence of excitation fields on vortex core dynamics in micron-sized magnetic disks\textsuperscript{1}. XIUEMEI CHENG, DAVID KEAVNEY, KRISTEN BUCHANAN, RALU DIVAN, Argonne National Laboratory — Magnetization vortices in micron-sized magnetic disks have been of great interest because of potential applications in memory devices. Theory predicts a rich spectrum of excitations including the fundamental or gyrotropic mode. Experimentally the gyrotropic mode is observed in some experiments while in others a linear or elliptical trajectory is seen. We have imaged free vortex core motion in permalloy disks of $6 \mu m$ diameter using time-resolved x-ray photoemission electron microscopy at beamline 4-ID-C of the Advanced Photon Source with 90 ps temporal resolution. We demonstrate that the vortex core motion trajectory depends on the magnitude of the excitation field. The vortex core exhibits a gyrotropic trajectory under low excitation fields, while under high excitation fields the core shows a more linear trajectory. We find that if the initial displacement of the core is greater than 20\% of the disk radius, transient magnetic domains appear in the first 1 ns after removal of field. These domain states then profoundly influence the subsequent motion. The core oscillation frequencies are consistent with theoretical predictions, regardless of the excitation amplitude.

\textsuperscript{1}Work was supported by the U. S. DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

1:39PM B32.00009 Direct Observation of Magnetic Vortex Cores using Scanning Electron Microscopy with Polarization Analysis (SEMPA), SEOK-HWAN CHUNG, CNST, NIST, Gaithersburg, MD 20899 / Maryland NanoCenter, University of Maryland, College Park, MD 20742, DANIEL PIERCE, JOHN UNGURIS, CNST, NIST, Gaithersburg, MD 20899 — Magnetic singularities associated with magnetic vortex cores are a common feature in patterned magnetic nanostructures. Their small size, on the order of 10 nm, makes them technologically interesting, but also difficult to measure or image directly. We used Scanning Electron Microscopy with Polarization Analysis (SEMPA) to image magnetic vortices in a wide variety of patterned nanostructures. Since SEMPA can measure both the in-plane and the out-of-plane component of the surface magnetization, SEMPA can potentially determine both the chirality and the polarity of the vortex core, simultaneously. Samples consisted of NiFe (25nm) / Ta (3nm), and other soft magnetic films, patterned by electron beam lithography and lift-off into disks with various diameters. The films were grown on 85nm thick SiN membranes to reduce image degradation from backscattered electrons. The experimental results were compared to micromagnetic simulations and the vortex core profile showed a good correspondence with theoretical predictions, which considers only the exchange and magnetostatic energy. This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement.

1:51PM B32.00010 Transition states of magnetization reversal in ferromagnetic nanorings, GABRIEL CHAVES-O'FLYNN, ANDREW KENT, DANIEL STEIN, New York University — Thin ferromagnetic rings are of interest for fundamental studies of magnetization reversal, in part, because they are a rare example of a geometry for which an analytical solution for the rate of thermally induced switching has been determined [1]. The theoretical model predicts the transition state to be either a global magnetization rotation of constant azimuthal angle or a localized fluctuation, denoted the instanton saddle. Numerically we have confirmed that for a range of values of external magnetic field and ring size the instanton saddle is energetically favored [2]. The model takes the annular width to be small compared to the mean radius of the annulus; in which case the main contribution to the magnetization energy comes from the surface magnetostatic energy. We present numerical micromagnetic calculations of the activation energy for thermally induced magnetization reversal for the two different transition states for the case when the annular width is equal in magnitude to the mean radius of the ring. Results of the total and surface magnetostatic energies are compared for different ring sizes. [1] K. Martens, D.L. Stein, A.D. Kent, PRB 73, 054413 (2006) [2] G.D. Chaves-O'Flynn, K. Xiao, D.L. Stein, A. D. Kent, arXiv:0710.2546 (2007)

2:03PM B32.00011 Probing a SET nanomagnet with shot noise, L.D. CONTRERAS-PULIDO, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain., J. FERNANDEZ-ROSSISSERT, Universidad de Alicante, Spain., R. AGUADO, Instituto de Ciencia de Materiales de Madrid, CSIC, Spain. — Although recent experiments show that single atomic spins [1] and molecular magnets [2] can be probed via transport measurements, their magnetic properties can hardly be tuned once they are fabricated. In a recent Letter [3], we have shown that a single-electron transistor (SET) based upon a 11-ML semiconductor quantum dot and doped with a single Mn ion behaves like a quantum nanomagnet with magnetic properties which can be controlled electrically. Conversely, the electrical properties of this SET depend on the quantum state of the Mn spin. Here, we extend these previous ideas and study the shot noise of this kind of nanomagnets. Our results reveal that shot noise contains much more information that the one contained in the average current. Interestingly, important quantities of the nanomagnet like the spin relaxation time and information about current-induced spin precession can be directly extracted from shot noise measurements. [1] Cyrus F. Hirjibehedin et al, Science, 317, 1199 (2007). [2] Moon-Ho Jo et al, Nanoletters, 6, 2014, (2006). [3] J. Fernandez-Rossier and R. Aguado, Phys. Rev. Lett. 98, 106805 (2007).

Monday, March 10, 2008 11:15AM - 2:03PM — Session B33 DMP GMAG FIAP: Focus Session: Spin Dependent Phenomena in Semiconductors: II Morial Convention Center 224

11:15AM B33.00001 Imaging Drift and Diffusion of Accumulation from the Spin Hall Effect\textsuperscript{1}. N.P. STERN, D.W. STEUERMAN, S. MACK, A.C. GOSSARD, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The spontaneous generation of spin polarization near sample edges by the spin Hall effect when electron currents flow in a metal or semiconductor with spin-orbit coupling has attracted recent attention due to the elegant and complex spin-orbit physics as well as the potential for all-electrical spin generation in spintronics devices. Optical techniques in semiconductors allow for spatial resolution of the electrically generated spin accumulation, a feature not present in all-electrical measurements. We use Kerr rotation microscopy to image the spatial and temporal evolution of spin accumulation produced by the extrinsic spin Hall effect in n-GaAs devices. Measurements in a variety of device geometries, including arms transverse to a channel, reveal the unambiguous contribution of longitudinal spin drift in accumulation profile.\textsuperscript{2} We develop one- and two-dimensional drift-diffusion modeling to explain the observed features, providing a more complete understanding of observations of spin accumulation and the spin Hall effect.

\textsuperscript{1}Work supported by NSF, ONR, and the Hertz Foundation.


11:27AM B33.00002 ABSTRACT WITHDRAWN

11:39AM B33.00003 Fractional Charge and Topological Pumping in the Quantum Spin Hall Insulators, TAYLOR HUGHES, XIAO-LIANG QI, SHOUCHENG ZHANG, Stanford University — We study the physics at the edge of a 2d topological (quantum spin Hall) insulator. This system is known to be topologically non-trivial and a profound manifestation of topologically non-trivial states of matter is the occurrence of fractional charge. In this work, we show that a magnetic domain wall at the edge of the quantum spin Hall insulator carries one half of the unit of electron charge, and we propose an experiment to directly measure this fractional charge on an individual basis. As an additional consequence, a rotating magnetic field can induce a topologically pumped dc electric current, and vice versa. Finally, we discuss an interacting version of this model in which the fractional charge is carried by the fundamental excitations. These physical phenomena can be derived from a generic topological effective action for topological insulators and are directly related to the physics of the second Chern number as will be described in another talk.
that the Anderson localization-delocalization transition between the metallic and insulating phases belong to the conventional symplectic universality class $Z_2$. Extensive numerical calculations indicate that the two models have exactly the same universal QSHE conductance fluctuation value $\pi/2$. This is confirmed by the analytical solution for a hard-wall boundary, which also yields the detailed distribution of the local spin polarization. The latter shows a universal distribution rather than a Gaussian distribution. Our results strongly suggest that the quantized spin-Hall conductance fluctuation belongs to a new universality class.

in the spectral distribution of the local spin density. Fast (Friedel) oscillations with the spin-orbit coupling entering via the period of slow beatings only. Long-wavelength contributions of evanescent and normal modes exactly cancel each other in the spectral distribution of the local spin density. The result is confirmed by the analytical solution for a hard-wall boundary, which also yields the detailed distribution of the local spin polarization. The latter shows a universal distribution rather than a Gaussian distribution. Our results strongly suggest that the quantized spin-Hall conductance fluctuation belongs to a new universality class.

1:03PM B33.00010 Network Model for $Z_2$ Quantum Spin-Hall Effects with Disorder, HIDEAKI OBUSE, AKIRA FURUSAKI, RIKEN, Japan, SHINSEI RYU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CHRISTOPHER MUDRY, Paul Scherrer Institute, Switzerland — We study the effects of static disorder on the $Z_2$ quantum spin-Hall effect for noninteracting electrons on the propagation of noninteracting electrons subjected to spin-orbit couplings with the time-reversal symmetry. This network model is different from past network models belonging to the symplectic symmetry class in that the propagating modes along the links of the network has a single Kramers doublet. By investigating this network model numerically, it is found that a two-dimensional metallic phase of finite extent is embedded in insulating phases. We also find that the Anderson localization-delocalization transition between the metallic and $Z_2$ insulating phases belong to the conventional symplectic universality class in two dimensions.
and challenges of UNCD-electronics, which will be discussed, are (a) the possibility of controlled doping of these films, (b) the influence of doping on chemical and ferromagnetic ring nanodevices. A brief discussion and

1:15PM B33.00011 Intrinsic spin-Hall effect in the presence of an in-plane magnetic field\(^1\), LUYAO WANG, CHONSAAR CHU, National Chiao Tung University, ANATOLY MALSHUKOV, Russian Academy of Sciences, Institute of Spectroscopy — The intrinsic spin-Hall effect (SHE) induced by a driving electric field \(E_x\) in the presence of an in-plane magnetic field \(\vec{B}\) in a 2D semiconductor strip is studied. In the diffusive regime, the spatial distribution of spin densities \(S_i(x=\pm x_0, y)\) is calculated from a spin diffusion equation derived from nonequilibrium Green’s function. For the case of Rashba spin-orbit interaction (SOI), we find that the spin polarization \(S_x\) normal to the 2D strip remains zero with or without the in-plane magnetic field. For the case of Dresselhaus SOI, where cubic term is included, the symmetry of \(S_x\) with respect to the in-plane magnetic field depends on the orientation of the \(\vec{B}\) field. With \(\vec{B}\) along \(x\), \(S_x\) exhibits symmetric dependence on \(B_z\). However, with a transverse in-plane magnetic field, along \(y\), at the edge of the strip exhibits asymmetric dependence on \(B_y\). These results lead to a possible diagnostic tool for the identification of the SOI in the system.

\(^1\)National Science Council of ROC, NSC95-2112-M-009-004.

1:27PM B33.00012 Phase transition between quantum spin Hall and ordinary insulating phases, SHUCHI MURAKAMI, Tokyo Institute of Technology and PRESTO, JST, SATOSHI ISO, KEK, YSHAI AVISHAI, Ben-Gurion University and RTRA project, LPS and CEA, MASARU ONODA, CERC, AIST and CREST, JST, NAOOTO NAGAOCHA, University of Tokyo, CREST, JST, and CERC, AIST — We theoretically study the phase transition between the quantum spin Hall (QSH) and insulator phases, which involves a change of the \(Z_2\) topological number. We deal with 2D and 3D systems without impurity and interaction. We introduce a parameter \(m\) controlling the phase transition, and we study whether the gap closes or not by one-parameter tuning. In general, level repulsion prevents the gap from closing. In fact, the physics of the \(Z_2\) topological number is encoded in the problem whether the gap closes by tuning a single parameter. In 2D \([1]\), as well as in the 3D inversion-symmetric systems \([2]\), the gap closes at one point, \(m = n_0\), whereas in 3D inversion-asymmetric systems \([2]\), there appears a finite regime for \(m (n_1 < m < n_2)\) showing a gapless phase between the QSH and insulator phases. In the gapless phase the monopoles and antimonopoles exist in the \(k\)-space, and they annihilate in pair at the gap opening. Implications of the present results to real materials \([3]\) are discussed. \([1]\) S. Murakami et al., Phys. Rev. B76, 205304 (2007). \([2]\) S. Murakami, New J. Phys. 9, 356 (2007). \([3]\) S. Murakami, Phys. Rev. Lett. 97, 236805 (2006).

1:39PM B33.00013 A voltage probe of the spin Hall effect\(^1\), YURIY PERSHYN, MASSIMILIANO DI VENTRA, Department of Physics, University of California, Santa Barbara, California 93106, USA — The spin Hall effect does not generally result in a transverse voltage. We predict that in systems with inhomogeneous electron density in the direction perpendicular to the main current flow, the spin Hall effect is instead accompanied by a transverse voltage. We find that, unlike the ordinary Hall effect, this voltage is quadratic in the longitudinal electric field for a wide range of parameters accessible experimentally. We also predict spin accumulation in the bulk and sharp peaks of spin Hall induced charge accumulation near the edges. Our results can be readily tested experimentally, and would allow the electrical measurement of the spin Hall effect in non-magnetic systems and without injection of spin-polarized electrons.

\(^1\)This work is partially supported by NSF Grant No. DMR-0133075.

1:51PM B33.00014 Spin-charge Separated Excitations in a Topological Insulator, DUNG-HAI LEE, YING RAN, ASHVIN VISHWANATH, University of California, Berkeley — We construct a simple, controllable, two dimensional model based on a topological band insulator. It has many attractive properties. The main conclusions are: (1) The quasiparticles exhibit spin-charge separation. (2) It suggests an alternative way to classify \(Z_2\) topological insulator without resorting to the sample boundary. (3) The quasiparticle condensation triggers a phase transition from a spin liquid to an insulating easy-plane ferromagnet.

Monday, March 10, 2008 11:15AM - 1:39PM — Session B35 FLAP: Focus Session: Emerging Materials and Devices I Morial Convention Center

11:15AM B35.00001 The Nanoelectronics Research Initiative and Beyond CMOS Research Activities in the US, GEORGE I. BOURIANOFF, Intel — The six leading Semiconductor Companies in the US have joined forces with Federal and State government to form the Nanoelectronics Research Initiative in 2005. The goal is to find new information processing paradigms, systems and devices which will extend Moore’s Law functional scaling into the indefinite future. The research activities are guided by 5 central research vectors which define the scope and content of the program and are listed below.

1. Computational state variables other than electronic charge
2. Non-equilibrium systems out of equilibrium with the thermal environment
3. Novel information transport mechanisms
4. Nanoscale thermal management
5. Directed self assembly of complex heterostructures

The current NRI research effort consists of 56 projects at 25 universities and 3 research centers in a coherent program where each project is aligned with one or more of the research vectors. During the past two years, significant progress has been made in a number of areas including spin wave, generation, detection and characterization, room temperature DMS materials, femtosecond magnetic domain switching characterization, improved MQCA structures, multiferroic and, magnetoelectric materials and devices, non-conformational metal insulator phase transitions in \(\mathrm{ VO}_2\) and ferromagnetic ring nanodevices. A brief discussion and references will be provided.

11:51AM B35.00002 Diamond Nanoelectronics\(^1\), IGOR ALTFEDER, Air Force Research Laboratory, JACQUELINE KRIM, North Carolina State University, ANDREY VOEVODIN, Air Force Research Laboratory — Thin films of ultra-nanocrystalline diamond (UNCD) represent an extremely promising nanoelectronic material. The electronic devices based on UNCD can operate at temperatures exceeding by an order of magnitude the working temperature of silicon-based devices. This talk will describe the recent STM/AFM study of CVD-grown UNCD films. The most important advances and challenges of UNCD-electronics, which will be discussed, are (a) the possibility of controlled doping of these films, (b) the influence of doping on chemical structure of UNCD surfaces and interfaces, and (c) exploring extremely low surface adhesion/friction of UNCD for design of MEMS.

\(^1\)Research supported by AFOSR/MURI.
12:03PM B35.00003 Low frequency Noise in Top-Gated Ambipolar Carbon Nanotube Field Effect Transistors. GUANGYU XU, Department of Electrical Engineering, University of California at Los Angeles (UCLA), FEI LIU, IBM T. J. Watson Research Centers (IBM), SONG HAN, UCLA, KOUNGMIN RYU, Department of Electrical Engineering, University of Southern California (USC), ALEXANDER BADMAEV, CHONGWU ZHOU, USC, KANG L. WANG, UCLA, UCLA TEAM, IBM TEAM, USC TEAM — Low-frequency noise of top-gated ambipolar carbon nanotube field effect transistors (CNT-FET) with aligned CNT growth onto the quartz substrate is presented. The noise of top-gated CNT-FETs in air is lower than that of back-gated devices, and is comparable with that of back-gated devices in vacuum. This shows that molecules in air act as additional scattering sources, which contribute to the noise. Different noise amplitudes in the electron-conduction region and hole-conduction region are due to both the Schottky barriers (SB) with respect to the conduction band and valance band and the scattering in the channel. The SB contact determines the sample conductance, and thus the noise; the channel scattering also determines the noise. The impact of channel length to the noise amplitude is discussed. This device offers a potential low noise CNT-FET structure.

3Work supported by DARPA and AFOSR.

12:15PM B35.00004 Nanopositioning of Individual Vertical Aligned Carbon Nanotubes on Interconnects. REGINALD C. FARROW, AMIT GOYAL, SHENG LIU, ZAFAR IQBAL, GORDON A. THOMAS, New Jersey Institute of Technology, LINUS A. FETTER, Bell Laboratories — Electrophoresis has been used to deposit single wall carbon nanotubes in arrays of sub-100 nm windows in insulating thin films over metal interconnects. The number of nanotubes that are deposited depends on the electric field and the geometry of the windows and nanotubes. Surface charge on the insulator causes the windows to become nanoscopic electrostatic lenses. Under certain readily achievable conditions only one nanotube will be deposited at the base of a window since each deposited nanotube modifies the electric field. This discovery enables the process integration of vertical aligned carbon-based electronics with more traditional technologies such as complementary metal oxide semiconductor (CMOS) using the current generation of lithography and process technology. Devices such as vertical field effect transistors and interconnected nanopore arrays may now be fabricated in the metal levels of CMOS integrated circuits to facilitate three-dimensional polyhilitic circuit architectures.

3Work supported by DARPA and AFOSR.

12:27PM B35.00005 Impact Ionization in Photocurrent Measurements of Carbon Nanotube p-n Junctions. NATHANIEL GABOR, Lab of Atomic and Solid State Physics, Cornell University, Z. ZHONG, LASSP, Cornell U., K. BOSNICK, Natl Inst for Nanotech, Natl Research Council of Canada, J. PARK, Chem. and Chem. Biology, Cornell U., P.L. MCEUEN, LASSP, Cornell U. — We investigate the photocurrent response at a nanotube gated p-n junction using a focused laser illumination source. Scanned photocurrent imaging demonstrates that photocurrent response occurs primarily in the p-n junction. Measurements in an optical cryostat down to 4K reveal large photoresponse and unusual step-like structure in the reverse bias photocurrent. We relate the intersection point of the forward bias photocurrent to the flat band condition in the device and infer the band gap, which is in excellent agreement with the band gap determined by thermal activation and diameter measurements. The striking photocurrent steps in reverse bias occur at intervals roughly equal to the band gap. We attribute these steps to impact ionization and carrier multiplication in the junction region of the device. By measuring the photon energy dependence of the impact ionization process, we determine that ionization occurs with high probability for carriers in the second and higher subbands of carbon nanotubes. These results show that nanotube p-n junctions provide an ideal system for probing carrier dynamics and interactions of electrons and holes in nanotubes.

12:39PM B35.00006 High Performance Silicon Nanowire Field Effect Transistor. QILIANG LI, Professor of Electrical Engineering, George Mason University, XIAOXIAO ZHU, YANG YANG, DIMITRIS IOANNOU, JOHN SUEHLE, CURT RICHTER — We report the fabrication and characterization of double-gated Si nanowire field effect transistors with excellent electrical characteristics and a small subthreshold slope: ~ 85 mV/dec. The Si nanowires were grown by chemical vapor deposition at pre-defined location on a 50 nm thermal SiO$_2$ (bottom gate oxide). The source/drain electrodes (Al) were formed by using photolithographic alignment and metal lift-off processes. A thin layer of SiO$_2$ was deposited on the HfO$_2$ as a buffer layer before the top gate electrode formation (Al, using photolithographic and lift-off processes). This self-aligned process enables the integration of a large number of high-quality nanowire transistors for electronic circuitry. We have investigated the effect of device structure and annealing conditions on the final device performance, and developed theoretical models to assist the device optimization.

1We acknowledge the support of the NIST Office of Microelectronics Programs and Semiconductor Electronics Division.

12:51PM B35.00007 Effects of Non-Ideal Edges in Graphene Nanoribbons. D. BASU, M.J. GILBERT, L.F. REGISTER, S.K. BANERJEE, Microelectronics Research Center, The University of Texas at Austin, A.H. MACDONALD, Department of Physics, The University of Texas at Austin — We report quantum mechanical transport simulations of the edge effects of nanoribbons of two-dimensional (2D) graphite sheets or graphene. Semiconducting graphene nanoribbons have the potential to augment Si technology because of their excellent electronic properties. In practice we find that scattering from the vacant sites in an otherwise perfect armchair edge of graphene reduces its transmission characteristics drastically. These effects decrease as the widths of the ribbons increase and as the number of steps along the edges decrease. However, band gap of these semiconducting graphene decreases as the width increases, leading to an increase in the band-to-band leakage current. We conclude that without atomic precision to define perfect edges, it may not be practical to use very narrow graphene layers as a semiconducting material for field effect transistors (FETs). Our tight-binding treatment of vacancies allows us to study not only FET-like devices, but also the effect of disorder that breaks symmetry in the graphene sheet for more exotic applications such as pseudospin-type devices.

1This work was supported in part by the NRI SWAN Center, DARPA and by SRC.

1:03PM B35.00008 Determination of Non-Accumulative Effects in PCMO Resistive Switches. STEPHEN TSUI, NILANJAN DAS, Y.Q. WANG, Y.Y. XUE, Texas Center for Superconductivity at the University of Houston, C.W. CHU, Hong Kong University of Science and Technology, Technology Center for Superconductivity at the University of Houston, Lawrence Berkeley National Laboratory — In recent years, the observation of electric field induced resistive switching occurring at the interface between a Ag electrode and Pr$_{0.7}$Ca$_{0.3}$MnO$_3$ (PCMO) thin film has stirred a great deal of activity. The controllable switching, depending on the applied voltage polarity, associated with this and other perovskite oxide systems may very well be a means to develop new nonvolatile memory devices. However, a consensus has not yet been reached on the origins of the physical mechanism, be it lattice rearrangement, electromigration, charge trapping, or carrier doping. An important issue is whether the switching behaves in an accumulative fashion, e.g. driven by a change in oxygen stoichiometry through ion-migration. We explore the situation through transport properties, switching characters and the size dependence of the switching area. Our results indicate that a large scale accumulation driven mechanism is not likely for the switching and that a local structural rearrangement may be a more reasonable physical process.
1:15PM B35.00009 A Physical Model for Resistive Switching In Metal-Oxide Interface, NILANJAN DAS, STEPHEN TSUI, YURI WANG, YUJU XUE, Department of Physics, University of Houston and TCSUH, CHING-WU CHU, Department of Physics, University of Houston, TCSUH, LBNL, California and HKUST, Hong Kong — Resistive switching in metal-oxide interfaces has been studied extensively and different models have been proposed. We have investigated the switch in metal-PMO (Pr$_{0.7}$Ca$_{0.3}$MnO$_3$) sample. Interface R and C, both have been found to be frequency independent almost up to 10 MHz. Also the activation energy for both the states (High and Low) are almost the same with bulk as found in R(T) plot. The physical picture will be very shallow potential wells, which may not be enough for retention observed. A pure electronic process (trapping and de-trapping in defects) of carrier only, as suggested earlier, will not be correct answer.

1:27PM B35.00010 Percollative model for resistance switching, S. H. CHANG, S. C. CHAE, J. S. LEE, S. B. LEE, Seoul National University, D.-W. KIM, Hanyang University, B. KHANG, T. W. NOH, Seoul National University — There have been research efforts on resistive switching in numerous insulating oxide films for the next nonvolatile memory device. Recently percolation has been considered as a key concept to explain unipolar memory switching [1]. The rupture process of conducting path is closely related to thermal heat budget induced by Joule-heating effect. In this process, the thermal heat dissipation during rupture could play important role in details of unipolar memory switching. In this study, we investigated correlation between the resistance switching behaviors of Pt/NiO/Pt capacitor structures and thermal heat dissipation as a function of the bottom electrode and temperature. Our modified percolative simulation and finite element analysis demonstrated these phenomena. [1] S. C. Chae et al., Adv. Mat., to be published (2007).

Monday, March 10, 2008 11:15AM - 1:39PM —
Session B36 GIMS: Focus Session: Advances in Scanned Probe Microscopy I: Low Temperatures
Morial Convention Center 228

11:15AM B36.00001 Subkelvin spin polarized STM: measuring magnetization curves of individual adatoms, JENS WIEBE, Institute of Applied Physics, University of Hamburg — Magnetic nanostructures consisting of a few atoms on non-magnetic substrates are explored as model systems for miniaturized data storage devices and for the implementation of novel spin-based computation techniques. Since these nanostructures are well defined and controllable on the atomic scale, they are ideally suited to study the fundamentals of magnetic interactions. We used spin polarized scanning tunneling spectroscopy at subkelvin temperatures to image the magnetization of individual adatoms as a function of an external magnetic field. This allows to directly measure their magnetic interactions at very low energy scale. We will present the design of the 300mK STM [1] and then focus on the results. Interestingly, Co atoms on Pt(111) behave paramagnetic even at very low temperatures. 300 times smaller than the previously reported giant barrier between up and down spin [2]. A peculiar variation in the saturation flux density, which is measured for each atom, is found. This is attributed to their mutual indirect exchange via the substrate electrons. Indeed, we observe an interaction between the adatom and a Co monolayer stripe oscillating with distance between ferromagnetic and antiferromagnetic coupling on the scale of the Fermi wavelength.


11:51AM B36.00002 Investigation of Acceptor States and Landau Levels in (In,Mn)As by Scanning Tunneling Spectroscopy, YOUNG JAE SONG, NIST-CNST/UMD-NanoCenter, NIKOLAI ZHITENEV, JOSEPH STROSCIO, Center for Nanoscience and Technology, NIST, Gaithersburg, MD, GREGORY RUTTER, PHILLIP FIRST, Georgia Tech., Atlanta, GA — Increased interest in spin-based electronics as a replacement for charge-based electronics has led to significant scientific attention on dilute magnetic semiconductors (DMS). Magnetically doped III-V semiconductors are a strong research focus, with the aim of achieving higher Curie temperatures by understanding the microscopic nature of ferromagnetism in these DMS materials. In this presentation, we discuss our recent study of single Mn acceptor states in InAs(110). Mn impurities deposited at low temperature are substituted by using STM atom manipulation techniques to exchange a Mn atom with a surface In atom [1]. Voltage-dependent imaging and scanning tunneling spectroscopy (STS) reveal a number of electronic states associated with the Mn acceptor state and the Landau levels in the 2D subbands of an accumulation layer as a function of applied magnetic field. This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement, NSF grant ECS-0404084, and Dept. of Commerce/NIST grant 60NANB7D6166. [1] Dale Kitchen et al, Nature 442, 436 (2006).

12:03PM B36.00003 Atomic manipulation and tunneling spectroscopy on vacancy of Ag(111) surface studied with LT-STM, DANDA P. ACHARYA, KAI F. BRAUN, SAW W. HLA, Ohio University — The evolution of the surface state and the effect of vacancies on the Ag(111) surface are investigated at an atomic scale by combining scanning tunneling microscopy and spectroscopy and atom manipulation at 5 K. Various vacancy sizes, from one atom to hundreds of atoms, on Ag(111) are first created by tip-sample contact in a controlled manner. Using lateral manipulation, a vacancy is filled one at a time and the corresponding differential conductance spectra are recorded. Small energy shifts in the onset of surface state are observed. The shift is more pronounced for small size vacancy and becomes less and less pronounced for larger size vacancies. The observed dI/dV intensities at different size of vacancies clearly reveals that the surface state onset on Ag(111) disappears after reaching towards the 6th layers.

12:15PM B36.00004 Direct detection of force gradient using atomic force microscopy with very small oscillation amplitude, TOSHU AN, ATSUSHI NOMURA, TAKAHIRO NISHIO, TOYOAKI EGUCHI, KOTONE AKIYAMA, YUKIO HASEGAWA, The Institute for Solid State Physics, The University of Tokyo — Using a quartz, which has a self-sensing capability, simple configuration of atomic force microscopy (AFM) is realized, and because of its high stiffness frequency-modulation (FM) operations with a small oscillation amplitude below 100 pm is possible. The small amplitude AFM operation enhances sensitivity of short range forces. Moreover, a force gradient can be directly detected from force vs. distance measurements. We carried out FM-AFM at low temperature (LT) in ultra-high vacuum using a quartz length-extension resonator with a tungsten tip (Spring constant and resonant frequency of the resonator are 540 000 N/m and 1 MHz, respectively) (An et al., APL 76, 133114 ’05). The system was simply made by attaching an extra electrode to the tip-holder of our LT scanning tunneling microscope cooled by He (APL 88, 113115 ’06). Direct detection of the force gradient was performed on the Si(111) 7X7 surface using very small oscillation amplitude of 70 pm at 2.4 K.

1:PRESTO, Japan Science and Technology Agency
2:present address, Institute for Materials Research, Tohoku Univ.
12:27PM B36.00005 Low-Temperature Nanotribology of Au and Pb using a Quartz Tuning-Fork. CARLOS UNTIEDT, GIOVANNI SAENZ-ARCE, Depto. Fisica Aplicada. Universidad de Alicante. — Quartz Tuning-Fork (TF) has been in recent years successfully implemented in force detection schemes for scanning probe microscopy (SPM) applications. Here we report its use as a nanotribometer for measuring friction in atomic size areas. The idea behind such a friction detector, is to take advantage of the large Q-factor of a TF ($Q_{air} \sim 6000$, $Q_{vac} \sim 20000$ at room temperature) which in our set-up depends of the SPM tip-sample dissipative forces. We have measured the Q-factor and the resonance frequency for various TFs. As a first step in the use of a TF as a nanotribometer, we studied the reactive forces that are associated with the combined local elastic properties of the sample and tip and calculated the damping rate associate with changes of the tip-sample distance. Finally, we show the variation of the measured damping rate and local spring constants with tip-sample distances for Au and Pb. For the measurement we have used our TF-nanotribometer at different temperatures ranging from 1.5K to room temperature in high vacuum.

12:39PM B36.00006 A Nano-Scale Scanning SQUID Susceptometer for the Measurement of Isolated Magnetic Moments. NICHOLAS C. KOSHNICK, Stanford University, MARTIN E. HUBER, University of Colorado Denver, JULIE BERT, HENDRIK BLUMH, Stanford University, JEFFREY LARGE, HAL EDWARDS, Texas Instruments, KATHRYN A. MOLER, Stanford University — Superconducting Quantum Interference Devices (SQUIDs) are well known as excellent magnetic field sensors. We present a scanning DC SQUID susceptometer that is designed to couple well to nanometer-sized objects. Its gradiometric design and local field coils allow for cancellation of the applied field so that dynamic range issues do not limit the SQUID’s sensitivity. Integrated modulation coils linearize the signal and allow for optimal performance at all applied fields. Planar coaxial shielding, enabled by a multi-layer niobium process, results in a low inductance (100 pH) millimeter scale design where the pickup loops can be optimized independently from the junction and shunt resistor parameters. The sensor loop is on a terraced structure so that it can be scanned approximately 100 nm from the sample surface. Focused Ion Beam milling is used to fabricate pickup loops with inner diameters between 250 nm and 2 microns with line widths of approximately 200 nm. A white noise sensitivity of 0.8 $\mu$V/$\sqrt{Hz}$ gives an estimated spin sensitivity of 80 $\mu$G/$\sqrt{Hz}$ at 4 Kelvin. We will also report on on-going scanning susceptometry measurements, and on the spin sensitivity at low temperatures.

12:51PM B36.00007 Absolute in-situ calibration piezoelectric quartz tuning fork force Sensors. SANJAY BIDASARIA, Georgia Tech, ALEXEI MARCHENKOV, Georgia Tech, MARCHENKOV GROUP TEAM — A method has been developed for absolute calibration of piezoelectric quartz tuning forks for use as force sensors with nano-newton resolution. The performance of the forks in a cryogenic environment is investigated. The mechanical properties of the forks are extracted from the frequency dependent admittance and compared to the exact model of a vibrating cantilever in a helium atmosphere. The method is verified by simple application of calibrated point loads to the cantilever in vacuum.

1:03PM B36.00008 A UHV-LT-STM System for Optical Experiments1. DAVID R. DAUGHTON, DONGHUN LEE, JAY A. GUPTA, The Ohio State University — The combination of optical techniques and scanning tunneling microscopy (STM) provides insight into a diverse set of physical processes including surface chemistry, surface-photon interactions, and spin scattering in semiconductors. We present a novel cryogenic setup, ultrahigh vacuum STM which incorporates a manipulable, high numeric aperture lens, with sub-5 micron spot size, in proximity to the tunnel junction. Modifications to our microscope have been made to improve upon the 12.5 K base temperature and 10 pm tip stability. Our initial efforts are focused on studies of photo-chemical reactions and chemical identification by tip-enhanced Raman spectroscopy (TERS). UHV deposition techniques have been developed for a variety of molecules well suited for TERS studies including azulene, azobenzene, methylene blue, and C60. Electrochemically and chemically-etched Au and Ag are optimized for field enhancement with characterization by scanning electron microscopy and collection of the plasmon emission from the tip. Raman spectra have been collected from molecule-coated tips in vacuum to test the optical setup for TERS.

1:15PM B36.00009 Photon-induced Molecular Motion Probed by STM. JUN ZHANG, KEVIN KELLY, Rice University, TAKASHI SASAKI COLLABORATION, JAMES TOUR COLLABORATION — To understand the mechanisms of nanoscale motion and manipulation in true molecular machines, we have investigated fullerenes and fullerene-based derivatives with an eye towards the molecular rolling motion on surfaces. Assisted by scanning tunneling microscopy (STM), we have successfully observed several bi-functional reactions between the chemically stable recording layer and the external photonics and tunneling electron excitations. In particular, we investigated a fullerene dimer structure which included an azo-based linkage. This system demonstrated a mechanical switching by incident irradiation, due to the azo transformation between the "cis" and "trans" states. This is particularly exciting in true molecular machines, we have investigated fullerenes and fullerene-based derivatives with an eye towards the molecular rolling motion on surfaces.

1:27PM B36.00010 Using a Geophone for Vibration Cancellation in a STM. ALAN FANG, ZHANYEBEK ALPICHSHEV, AHARON KAPITULNIK, Stanford University — We demonstrate a method for using a geophone (velocity-sensitive vibration sensor) for reducing the vibration-induced tunnel current noise in a Scanning Tunneling Microscope (STM). Some simple analog circuitry compensates for the transfer function of the vibration-induced noise for the experimental setup. Almacel-Lucent — Study of the energy gap of the fractional quantum Hall effect (FQHE) in the second Landau level will be presented. Two symmetrically doped GaAs/AlGaAs quantum well samples with densities $n = 3.2 \times 10^{11}$ cm$^{-2}$ and $n = 2.8 \times 10^{11}$ cm$^{-2}$ with respective mobilities of $\mu = 28.3 \times 10^5$ cm$^2$/Vs and $\mu = 10.5 \times 10^5$ cm$^2$/Vs were studied. In the higher mobility sample, clear FQHE states are observed at filling factor $\nu = 5/2, 7/3, 8/3, 14/5, 11/5, 12/5, 16/7, and 19/7$. Some of the higher order FQHE states disappear in the lower mobility sample, and clear FQHE states are observed at $\nu = 5/2, 7/3, 8/3, 14/5, and 11/5$. The energy gaps of the FQHE states at $\nu = 5/2, 7/3$ and 8/3 in the higher mobility sample are found to exceed 500mK. The energy gaps of the $\nu = 5/2, 7/3$ and 8/3 states in the lower mobility sample are typically reduced by more than 50% in comparison. Our measured gap for $\nu = 5/2$ state, which is less than 1/5 of the theoretical gap, can be understood when the finite width correction and disorder broadening is taken into account. Evolution of the energy gaps with mobility shows that the even-denominator FQHE state at $\nu = 5/2$ is the most robust FQHE state in the second Landau level. In addition, the $\nu = 7/3$ and 8/3 states are unlikely to be the second Landau level analog of the Laughlin states at $\nu = 1/3$ and 2/3 in the lowest Landau level.

Monday, March 10, 2008 11:15AM - 2:15PM — Session B37 FIAP: FQHE in Higher Landau Levels Morial Convention Center 229

11:15AM B37.00001 Evolution of the Fractional Quantum Hall States in the Second Landau Level. H.C. CHOI, W. KANG, University of Chicago, S. DAS SARMA, University of Maryland, L.N. PFEIFFER, K.W. WEST, Alcatel-Lucent — Study of the energy gap of the fractional quantum Hall effect (FQHE) in the second Landau level will be presented. Two symmetrically doped GaAs/AlGaAs quantum well samples with densities $n = 3.2 \times 10^{11}$ cm$^{-2}$ and $n = 2.8 \times 10^{11}$ cm$^{-2}$ with respective mobilities of $\mu = 28.3 \times 10^5$ cm$^2$/Vs and $\mu = 10.5 \times 10^5$ cm$^2$/Vs were studied. In the higher mobility sample, clear FQHE states are observed at filling factor $\nu = 5/2, 7/3, 8/3, 14/5, 11/5, 12/5, 16/7, and 19/7$. Some of the higher order FQHE states disappear in the lower mobility sample, and clear FQHE states are observed at $\nu = 5/2, 7/3, 8/3, 14/5, and 11/5$. The energy gaps of the FQHE states at $\nu = 5/2, 7/3$ and 8/3 in the higher mobility sample are found to exceed 500mK. The energy gaps of the $\nu = 5/2, 7/3$ and 8/3 states in the lower mobility sample are typically reduced by more than 50% in comparison. Our measured gap for $\nu = 5/2$ state, which is less than 1/5 of the theoretical gap, can be understood when the finite width correction and disorder broadening is taken into account. Evolution of the energy gaps with mobility shows that the even-denominator FQHE state at $\nu = 5/2$ is the most robust FQHE state in the second Landau level. In addition, the $\nu = 7/3$ and 8/3 states are unlikely to be the second Landau level analog of the Laughlin states at $\nu = 1/3$ and 2/3 in the lowest Landau level.
We give numerical evidence that at $\nu_{\text{Hall}}$ states in the first excited Landau level including $1$ induce a partially or fully polarized superconducting state. Field theory for coexisting order parameters, and show that even if repulsion is smaller than that required for a Stoner instability, ferromagnetic fluctuations can be crucial to recent proposals of topologically protected quantum computation. Most schemes to determine the statistics of the quantum Hall quasiparticles rely on the Coulomb interaction. In this work we consider the finite thickness of the electrically polarized quasi-2D quantum confinement in three models: Zhang-Das Sarma, infinite square-well, and Fang-Howard potentials, respectively. We calculate overlap between the Laughlin (fillings $1/3$ and $1/5$) or Pfaffian (filling $1/2$) and the corresponding exact state, obtained by exact diagonalization, in the lowest, second, and third LLs as a function of the layer thickness. We find that the Pfaffian state becomes a nearly exact description of the physics at filling factor $1/2$ in the SLL for a finite value of thickness. We also show the comparative trends in the ground state energy and the excitation gap as a function of layer thickness, comparing among the first, second, and third LLs. We acknowledge support from Microsoft Q Project. [1] Das Sarma et al. PRL 94, 166802(2005)

Our high density $(n=10^{11}$cm$^{-2}$) and high mobility GaAs samples are of sufficient quality such that well-defined quantum Hall states are resolved at $\nu=8/3$, $5/2$, and $7/3$ in the bulk at low temperature. In particular, we have studied the impact of confining geometry design and the size of the qpc opening on the stability of higher order fractional states in the qpc.

12:15PM B37.00006 Confinement of Fractional Quantum Hall States, ROBERT WILLETT, MICHAEL MANFRA, KEN WEST, LOREN PFEIFFER, Bell Laboratories — The quasiparticles of certain exotic quantum Hall states in the first excited Landau level including $\nu=5/2$ and $\nu=12/5$ are believed to obey non-Abelian statistics. Manipulation of such quasiparticles is crucial to recent proposals of topologically protected quantum computation. Most schemes to determine the statistics of the quantum Hall quasiparticles rely on the manipulation of the correlated state in confined geometries. As a preliminary step in this direction, we report on the magnetic field and temperature dependences of transport through quantum point contacts (qpc’s) in the regime where the first excited Landau level is partially occupied in the confined region. Our high density $(n=4x10^{11}$cm$^{-2}$) and high mobility GaAs samples are of sufficient quality such that well-defined quantum Hall states are resolved at $\nu=8/3$, $5/2$, and $7/3$ in the bulk at low temperature. In particular, we have studied the impact of confining geometry design and the size of the qpc opening on the stability of higher order fractional states in the qpc.

12:27PM B37.00007 Fractional Quantum Hall Hierarchy and the Second Landau Level, PARSAN BONDERSON, Microsoft Station Q, J.K. SLINGERLAND, Dublin Institute for Advanced Studies — We generalize the Haldane-Halperin hierarchy picture to apply to non-Abelian fractional quantum Hall states, and propose trial wave functions to describe the observed Hall conductance plateaux in the second Landau level. These hierarchy states are constructed over the Moore-Read state, the expected description of the $\nu=5/2$ plateau, and thus all have electron pairing in the ground state and an excitation spectrum that includes non-Abelian anyons of the Ising model $\sigma$-vortex type.

12:39PM B37.00008 Edge States and Interferometers in the Pfaffian and anti-Pfaffian States, WAHEB BISHARA, California Institute of Technology, CHETAN NAYAK, Microsoft Station Q, UCSB — In this work we use two theoretical candidates for describing the $\nu=5/2$ Quantum Hall state, the Moore-Read Pfaffian and its particle-hole conjugate, to calculate the conductance of a two point contact interferometer in the weak tunneling regime. We invoke the appropriate edge theory and calculate the conductance as a function of temperature and voltage, and we establish the connection to the underlying bulk topological theory.
12:51PM B37.00009 Spectrum of Quantum Entanglement in Fractional Quantum Hall States

HUI LI, F.D.M. HALDANE, Princeton University — We present numerical studies of the bipartite entanglement in fractional quantum Hall (FQH) states. We partitioned the (spherical geometry) Landau-level orbitals into two hemispheres: the entanglement spectrum derived from the Schmidt decomposition \(|\psi = \sum \exp(-\beta r/2)|\psi_A^\alpha \otimes |\psi_B^\beta\rangle\), where \(|\psi_A^\alpha\) (or \(|\psi_B^\beta\rangle\) are orthonormal. The \(\beta\)s are “energy levels” of a system with thermodynamic entropy at “temperature” \(k_B T = 1\) equivalent to the entanglement entropy. The entanglement spectrum, i.e., the relation between the \(\beta\) and the quantum numbers that classify \(|\psi_A^\alpha\) (or \(|\psi_B^\beta\rangle\) serves as a “fingerprint” of the topological phase of the FQH state, and reveals much more information than just the entanglement entropy, a single number. The spectrum of, e.g., the 1/3 Laughlin state has far fewer levels than expected for a generic wavefunction, and its low-energy spectrum corresponds to that of a conformal field theory (CFT). We studied the wavefunctions that interolate between the Laughlin state and the ground state of a realistic Coulomb interaction potential at \(\nu = 1/3\): the generic number of levels is restored, but the low-lying CFT structure remains essentially unchanged. We also describe the interpolation between the Moore-Read state and the Coulomb interaction ground state at \(\nu = 5/2\).

1:03PM B37.00010 Model Wavefunctions For Non-Abelian Quasiparticles

B. ANDREI BERNEVIG, F.D.M. HALDANE, Princeton University — We present model wavefunctions for quasiparticle (as opposed to quasihole) excitations of the Zk parafermion sequence (Laughlin/Moore-Read/Read-Rezayi) of Fractional Quantum Hall states. These states satisfy two generalized clustering conditions: they vanish when either a cluster of \(k+2\) electrons is put together, or when two clusters of \(k+1\) electrons are formed at different positions. For Abelian Fractional Quantum Hall states (\(k = 1\)), our construction reproduces the Jain quasielectron wavefunction, and elucidates the difference between the Jain and Laughlin quasiparticle constructions. For two (or more) quasiparticles, our states differ from those constructed using Jain’s method. By adding our quasiparticles to the Laughlin state, we obtain a hierarchy scheme which gives rise to a non-abelian \(\nu = \frac{3}{2}\) FQH state.

1:15PM B37.00011 Jack Polynomials, Exclusion Statistics, and non-Abelian FQHE States at \(\nu = k/(km + r)^1\)

F. D. M. HALDANE, B. ANDREI BERNEVIG, Princeton University — We describe a general family of non-Abelian FQHE states at \(\nu = k/(km + r)\) with polynomial wavefunctions \(\prod_{i<j}(z_i - z_j)^m J_k^{(m)}(z_1, \ldots, z_N)\), where \(J_k^{(m)}\) is a symmetric Jack polynomial with negative (coprime) rational parameter \(\alpha = -(k+1)/(r-1)\), and \(\lambda\) is the “most compressed” \(\{k, r, N\}\)-admissible” partition. These polynomials are dominated by an occupation-number pattern maximally-obeying the generalized Pauli rule that no (consecutive) group of \(km + r\) orbitals contains more than \(k\) particles and \((m > 0)\) no group of \(m\) orbitals contains more than one. This exclusion rule defines a space of polynomials characterized by how they vanish as clusters of particle coordinates contract to a point. The edge of these FQHE states has a fractionally-quantized thermal Hall effect with \(e_{\text{eff}} = k/(km + r)\), derived from the exclusion rule. The \(r = 2\) family are the Laughlin, Moore-Read, and Read-Rezayi states, related to unitary conformal field theories. The \(r > 2\) families are related to non-unitary \(W_{k + 1 + r}^*\) cft, but (as polynomials) have well-defined quasi-hole propagators, which overcomes the principal objection to the proposition that non-unitary cft’s can describe FQHE states. The \(m = 1, r = k + 1\) set are a non-Abelian alternative construction of states at 2/5, 3/7, 4/9, \ldots.

1Supported in part by NSF MRSEC DMR02-13706.

1:27PM B37.00012 Searching for anyons in a realistic model of fractional quantum Hall liquids

ZI-XIANG HU, Zhi-Xiang Hu, Dept. Phys, ZheJiang Univ, PR China, XIN WAN, Dept. Phys, ZheJiang Univ, PR China, PETER SCHMITTECKERT, Institute of Condensed Matter Theory, University of Bonn — We study quasihole/particle excitations in a microscopic model of fractional quantum Hall liquids with long-range Coulomb interaction and an edge confining potential. We find with a local trapping potential quasihole/particle states can emerge from the Laughlin and the Moore-Read states. The presence of Abelian and non-Abelian quasiholes has a distinct effect on the corresponding edge spectra. The stability of quasiholes/particles depends on the detail of the confining potential and the trapping potential. We discuss the relevance of the calculation to the high-accuracy generation and control of individual anyons in potential experiments, in particular, in the context of topological quantum computing.

2Supported in part by NSF MRSEC DMR02-13706.

3Dept. Phys, Florida State Univ, NMF.

1:39PM B37.00013 Probing Non-Abelian Statistics in \(\nu = 12/5\) Quantum Hall State\(^1\)

KAM TUEN LAW, Brown University — The tunneling current and shot noise between two Fractional Quantum Hall edges in \(\nu = 12/5\) state in electronic Mach-Zehnder Interferometer with two quantum point contacts (QPCs) is studied. We show that the tunneling current and shot noise can be used to probe the existence of non-Abelian statistics in the \(k = 3\) Read-Rezayi state. More specifically, the dependence of the current on the Aharonov-Bohm flux in the Read-Rezayi state is asymmetric under the change of the sign of the applied voltage. This property is absent in the Laughlin states. Moreover the Fano factor can exceed \(3\). The dependence of the current on the applied voltage is exactly \(12.7\) electron charges in the \(k = 3\) Read-Rezayi state. This number is much greater than the maximum possible Fano factor in all Laughlin states and the Moore-Read state which was shwon previously to be \(e\) and \(3.2e\) respectively.

\(^1\)This work was supported by the National Science Foundation under Grant No. DMR-0544116.

1:51PM B37.00014 Effect of Landau Level Mixing on Braiding Statistics

STEVEN H. SIMON, Alcatel-Lucent Bell Labs — We examine the effect of Landau level mixing on the braiding statistics of quasiparticles of abelian and nonabelian quantum Hall states. While path dependent geometric phases can perturb the abelian part of the statistics, we find that the nonabelian properties remain unchanged to an accuracy that is exponentially small in the distance between quasiparticles.

2:03PM B37.00015 Studying topological order in quantum Hall states using entanglement entropy calculations

MASUD HAQUE, MPI-PKS Dresden, Germany, OLEKSANDR ZOZULYA, KARELJAN SCHOUTENS, University of Amsterdam, The Netherlands, ED REZAYI, California State Univ, Los Angeles, NICOLAS REGNAULT, Ecole Normale Superieure, Paris, France — We present calculations of the entanglement entropy in fractional quantum Hall (FQH) states. Calculating the entanglement entropy between spatially separated regions allows us to probe the topological order in Laughlin and Moore-Read states. The entanglement entropy is also found to be a sensitive indicator of quantum phase transitions between FQH and non-FQH states.

11:15AM B38.00001 Perturbed Angular Correlation Study of ZrSiO$_4$ and HfSiO$_4$, HERBERT JAEGGER, Miami University, SEAN MCBRIDE, Kansas State University — Time-differential perturbed angular correlation spectroscopy is a powerful technique to study short-range interactions between probe nuclei and host crystals. The technique requires a very low concentration of radioactive probe nuclei and relies on the probes substituting for atoms of the host crystal. We report on PAC measurements of synthetic zircon and hafnon using $^{181}$Ta-probes to study the EFG at Zr and Hf lattice-sites. The quadrupole coupling constants for both zircon and hafnon decrease linearly with increasing temperature. The slope of $\nu_Q$ vs. $T$ increases above 800°C (zircon) and 1100°C (hafnon) as a consequence of a change in the Zr-O and Hf-O coordination. We also observe a systematic reduction of the anisotropy value $\Delta_{22}$ that is correlated with the onset of the structural change. Changes in the anisotropy are usually related to dynamic interaction and can be due to nuclear decay after effects. In our case we believe that we see evidence of a trapped electronic defect, giving rise to a rapidly decaying high-frequency quadrupole interaction. At higher temperatures the defect detraps and no longer causes a reduction in the anisotropy.

11:27AM B38.00002 Stability and lattice dynamics of SiO$_2$ cristobalite, SINISA COH, DAVID VANDELBILT, Department of Physics and Astronomy, Rutgers University — Among the phases of SiO$_2$ are alpha and beta cristobalite. Despite early indications that the higher-temperature beta phase might be cubic (Fe3m), it is now accepted that it is in fact tetragonal (I42d), and that the experiments suggesting a cubic structure were averaging spatially or dynamically over tetragonal domains. Recently, Zhang and Scott (J. Phys. Cond. Matt. 19, 275201) suggested that the lower-temperature alpha phase, widely accepted to be tetragonal (P412121), might be an artifact in a similar way. With this motivation we investigate the energy landscape in the vicinity of cristobalite phases using first-principles calculations. We use the ABINIT implementation of density-functional theory in a plane-wave pseudopotential framework. We find that both the P412121 alpha and I42d beta phases are local minima, thus reinforcing that the identification of the alpha phase as belonging to the P412121 structure. We compute the frequencies of phonon modes at high-symmetry k-points in both structures and compare with experiment. We also identify a minimum-energy path connecting the alpha and beta phases through an intermediate orthorhombic phase (P212121), and find a surprisingly low barrier of ~5 meV per formula unit. We note that a simple rigid-unit mode picture gives a good rough description of these energetics, and we map out the minimum-energy path in the space of rigid unit rotations in a physically insightful way.

11:39AM B38.00003 First Principles Modeling of BaCeO$_3$: Stabilization of O Vacancies, JOSEPH BENNETT, ANDREW RAPPE, University of Pennsylvania — We use first-principles density functional theory (DFT) calculations to investigate the ground state structures of both BaCeO$_3$ (BC) and Pd-doped BC (BCP) perovskites of general formula ABO$_3$. The relaxed structures match closely with recent experimental scattering studies, and also provide a local picture of how the BC perovskite lattice accommodates Pd. Both stoichiometric and oxygen-deficient materials are considered, and structures with an O vacancy adjacent to each Pd are predicted to be favored. The oxidation state of Pd in each doped structure is investigated through a structural analysis, the results of which are supported by an orbital-resolved projected density of states. The local bonding environments around Pd as well as the electron fillings of atomic orbitals on Pd and its neighbors are examined. A particular focus is the character of the highest occupied molecular orbital (HOMO) and the few lowest unoccupied molecular orbitals (LUMO). These electronic states are compared with expectations based on crystal field splittings in the computed atomic geometries. The vacancy stabilization by Pd in BCP is explained through redox chemistry and lattice strain relief.

11:51AM B38.00004 Dynamical structure factor of LiF for all wave vector transfers: New results and insights1, Q. KOU, M.C. TROPAREVSKY, A.G. EGIULUZ(1), Univ. of Tenn.; MSTD-ORNL(2), B.C. LARSON, J.Z. TISCHLER, MSTD-ORNL(2), P. ZSCHACK, APS-ANL(3) — We report a theoretical-experimental investigation of the dynamical structure factor of LiF. The calculations are done within the TDLDA of time-dependent density functional theory; the measurements correspond to non-resonant inelastic x-rays scattering (NIXS) cross sections, obtained in absolute units. The TDLDA spectra contain one adjustable parameter: a “scissors-operator” shift of the conduction bands. This parameter is determined in view of the NIXS line shape for $q=6\AA^{-1}$ ($q//c111$). The TDLDA spectra display a non-trivial semi-quantitative agreement with the NIXS data, for all wave vectors (directed along the three high-symmetry directions); indeed, the line shape changes drastically from the coherente-response small-$q$ regime, to the incoherent-response large-$q$ regime. The picture of the excitations which emerges offers an alternative view relative to a seminal investigation involving an approximate solution of the Bethe-Salpeter equation; W. A. Caliebe et al. Phys. Rev. Lett. 84, 3907 (2000).

11:53AM B38.00005 Simulation of Li ion diffusion near electrolyte-metal interface – Li$_3$PO$_4$ and Li**, YAOJUN DU, XIAO XU, N.A.W. HOLZWARTH, Wake Forest U. — Motivated by recent technological interest in Li$_3$PO$_4$-based electrolytes developed at Oak Ridge National Laboratory for use in rechargeable solid-state batteries and other technologies, we have used first-principles modeling techniques to study Li ion diffusion near idealized interfaces between Li$_3$PO$_4$ and Li metal. Using the nudged elastic band method, migration energy barriers for Li ion diffusion across interfaces in different crystallographic directions are calculated for both vacancy and interstitiality mechanisms. Preliminary results find interface migration barriers as low as 0.2 eV and 0.26 eV for the vacancy and interstitiality mechanisms, respectively. This suggests that interface diffusion barriers are likely to be comparable or lower than the corresponding migration barriers within crystalline Li$_3$PO$_4$.

12:03PM B38.00006 QNS study on superprotonic conductor, YUTAKA IKEDO, Toyota CRDL, HIROSHI NOZAKI, MASAHIKO HARADA, JUN SUGIYAMA, TAKU SATO, YASUMITSU MATSUO, YIMING QIU, JOHN COPLEY — Cesium hydrogen selenate, CsHSeO$_4$, and related materials M(H)X$_2$O$_4$, where M = Cs, Rb, K and X = S, Se, are considered to be a promising candidate as electrolyte materials for fuel cells. In order to clarify the mechanism of their high proton conductivity, quasielastic neutron scattering (QNS) measurements were carried out using single crystal samples of CsHSeO$_4$ on disk chopper spectrometer (DCS) in NIST Center for Neutron Research at temperatures mainly above T$_C$ (401 K), at which CsHSeO$_4$ undergoes a structural phase transition from a low-T orthorhombic phase (Phase II) to a high-T tetragonal phase (Phase I). High proton conductivity, i.e., super-protonic ionic conductivity is observed only in Phase I. The analysis of the QNS spectrum suggests an anisotropic proton diffusion in Phase I, in spite of the isotropic behavior reported by AC conductivity measurements. The present QNS result thus provides crucial information on the proton diffusion pass in these materials.

1 supported by NSF ITR Grant No. DMR-0219332; 2 sponsored by the DOE-BES, Div. of Materials Sciences and Engineering; 3 sponsored by the DOE Office of Science

12:15PM B38.00006 QNS study on superprotonic conductor, YUTAKA IKEDO, Toyota CRDL, HIROSHI NOZAKI, MASAHIKO HARADA, JUN SUGIYAMA, TAKU SATO, YASUMITSU MATSUO, YIMING QIU, JOHN COPLEY — Cesium hydrogen selenate, CsHSeO$_4$, and related materials M(H)X$_2$O$_4$, where M = Cs, Rb, K and X = S, Se, are considered to be a promising candidate as electrolyte materials for fuel cells. In order to clarify the mechanism of their high proton conductivity, quasielastic neutron scattering (QNS) measurements were carried out using single crystal samples of CsHSeO$_4$ on disk chopper spectrometer (DCS) in NIST Center for Neutron Research at temperatures mainly above T$_C$ (401 K), at which CsHSeO$_4$ undergoes a structural phase transition from a low-T orthorhombic phase (Phase II) to a high-T tetragonal phase (Phase I). High proton conductivity, i.e., super-protonic ionic conductivity is observed only in Phase I. The analysis of the QNS spectrum suggests an anisotropic proton diffusion in Phase I, in spite of the isotropic behavior reported by AC conductivity measurements. The present QNS result thus provides crucial information on the proton diffusion pass in these materials.

1 supported by NSF Grants DMR-0405456 and 0427055.


12:27PM B38.00007 Proton Transport in Mixed Rare-Earth/Alkaline Earth Metaphosphate Glasses1, GABRIEL HARLEY, UC Berkeley/Lawrence Berkeley National Laboratory/Max Planck Institute (FKF), LUTGARD C. DE JONGHE, UC Berkeley/Lawrence Berkeley National Laboratory — The transport properties of [La$_{1-x}$M$_x$]$_2$P$_2$O$_7$ metaphosphate glasses, where M is Ba, Sr, Ca, and $0.0 < x < 0.8$ were investigated in the 300 – 500 °C range. Protons are found to be incorporated as charge compensation for the substituting divalent cation. A model for proton conduction in phosphate glasses is presented where aliovalent cations within the phosphate network act as trapping sites for protons. Protons are transported via trapping center to trapping center along phosphate tetrahedra. The diffusion of protons is found to be between $10^{-8}$ cm$^2$/s and $10^{-6}$ cm$^2$/s in the 300–500 °C range. The conductivity increases two orders of magnitude from the unsubstituted to the 60% substituted glass reaching a maximum conductivity of $10^{-6}$ S/cm at 450 °C. The average transport distance between proton centers predicted by the electrical analysis is on the order of tens of nanometers, which is the same magnitude of proton-proton distance calculated from the structural data. The activation energy is found to be independent of concentration though dependent on modifying substitutional cation, and increases from 0.92 eV for Ba to 1.02 for Sr.

1Supported by the U.S. DOE-BES and by the Max Planck Institute

12:39PM B38.00008 Evidence of structure dependence of hyperpolarizability in octupolar molecules, CLAUDIA CARDOSO, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, PAULO ABREU, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, FERNANDO NOGUEIRA, CFC, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra — It was recently reported that second-order hyperpolarizability increases significantly upon introduction of positive charges at the pyridyl end groups in tripyridyl octopolar chromophores, when compared with the neutral species. We performed ab-initio and semi-empirical calculations for the geometries, electronic localization function and first hyperpolarizabilities of a series of 6 tripyridyl molecules in neutral and protonated forms. Ab-initio calculations correctly reproduce the large hyperpolarizability values of the protonated octopolar molecules. Semi-empirical calculations predict somehow smaller hyperpolarizability values but reproduce the trend of the experimental and ab-initio values. Linear response TDDFT calculations are in good agreement with the experimental absorption spectra, reproducing the red-shift of the peaks with protonation. A correlation between the molecular structures and the first hyperpolarizability was established.

12:51PM B38.00009 UV Spectra of rutile and anatase phases of TiO$_2$ using ABINIT2NBSE1, H.M. LAWLER, J.J. REHR, U. Washington, S. DALOSTO, Z.H. LEVINE, E.L. SHIRLEY, NIST — We have developed an interface between the electronic structure code ABINIT and the optical spectroscopy code NBSE developed at NIST. NBSE calculates dielectric spectra at various levels of theory, including iterative solution of the Bethe-Salpeter equation (BSE) for electron-hole states. From a single input file the interface executes a complete calculation, from the self-consistent ground-state to the dielectric spectrum. The interface can also treat momentum-transfer dependence of the dielectric function. As an application, we present calculations of the birefringent spectra of rutile and anatase TiO$_2$. Not surprisingly, we find that excitonic interactions dominate low-energy features of the spectra. We also address the role of planar-bonding, oxygen π-orbitals near the Fermi level, and the unfilled titanium d-band in the birefringent properties of these systems.

1Supported by DE-FG03-97ER45623

1:03PM B38.00010 Zeeman Effect in TiO$_2$:Cr$^{3+}$, MICHAEL CRAWFORD, DuPont Company, XING WEI, STAN TOZER, National High Magnetic Field Laboratory — We will describe the results of Zeeman effect measurements for single crystals of rutile TiO$_2$ doped with Cr$^{3+}$. These measurements, performed at the National High Magnetic Field Laboratory in magnetic fields with strengths up to 45 T, utilized the near-infrared luminescence of Cr$^{3+}$ at a temperature of T = 14 K. The Cr$^{3+}$ luminescence spectra show the evolution with field strength of the splitting of the Cr$^{3+}$ zero-phonon line at 12,684 cm$^{-1}$ in magnetic fields applied parallel or perpendicular to the crystallographic c-axis. In the former case the zero-phonon line splits into four Zeeman components, while for the latter case three components appear. These results will be discussed and compared to earlier measurements made in weaker magnetic fields.

1:15PM B38.00011 Raman elastic paramagnetic resonance (Raman-EPR) of Cr$^{3+}$ in ruby1, X. LU, Purdue University, S. VENUGOPALAN, SUNY, Binghamton, HYUNJUNG KIM, Sogang Univ. Korea, M. GRIMSDITCH, Argonne National Lab, S. RODRIGUEZ, A.K. RAMDAS, Purdue University — We have observed the Raman-EPR of the Zeeman split $^4A_2$ ground state of the Cr$^{3+}$ ion in Al$_2$O$_3$ :Cr, i.e., ruby, exploiting the resonance conditions associated with the R$_1$ line. Employing a tunable dye laser with a photon energy $E_Z$ in the vicinity of the Zeeman components of the R$_1$ luminescence, we observe the Stokes and anti-Stokes Raman transitions with shifts corresponding to the intra $^4A_2$ ground state level splitting by the external magnetic field (B). The proximity of the incident and the scattered radiation to the Zeeman components of R$_1$ leads to selective dramatic resonance enhancements of the intensities of EPR transitions brought about as a function of B and $E_Z$. The microscopic mechanism for the resonance enhancement involves the ‘in resonance’ and ‘out resonance’ conditions fulfilled by the virtual transitions from the sublevels of $^4A_2$ ground state to the sublevels of $^4E$ by the incident and the scattered radiation in a two step process. Raman-EPR of the Zeeman sublevels of $^4E$ excited state of R$_1$ is also observed.

1Work supported by NSF (DMR 0405082 and 0705783).

1:27PM B38.00012 Trivalent chromium probes in mixed dicyanoargentate-dicyanoaurate single crystals, C.L. LAROCHELLE, J.K. KREBS, Franklin & Marshall College — Single crystals of the form R[M(CN)$_3$]$_3$ (R=trivalent ion, such as a rare earth; M=Ag, Au, or both) have a layered structure consisting of alternating layers of M(CN)$_3$ ions and R$^{3+}$ ions. Recent work on this type of crystal has focused on energy transfer from the metal dicyanide donor to the rare earth acceptors, specifically Tb$^{3+}$, Eu$^{3+}$, Sm$^{3+}$, and Ce$^{3+}$. Crystals of this type are particularly interesting because the luminescence energies are tunable, changing with changes in the temperature as well as Ag/Au ratio. Doping these single crystals with chromium can provide an opportunity to study the crystal field strength at the ion site because the energy levels in chromium are very sensitive to the ion’s environment. We present steady-state excitation and emission results, along with lifetime measurements for a series of crystals of the type C$_6$H$_5$-Ar$_9$[Ag$_{1-x}$Au$_x$(CN)$_3$]$_3$, with $x=1, 0.5, 0.75, 0.9$. These measurements indicate that the chromium emission is of an unusually low energy in these crystals.

1:39PM B38.00013 Ce:Cr:YAG Based Yellow/Red Phosphors, JINKE TANG, WENDONG WANG, University of Wyoming, SHENG TENG HSU, Sharp Laboratories of America, BRIAN SULLIVAN, University of Wyoming — Ce:YAG (yttrium aluminum garnet) is the current industrial material of choice for phosphor for white LEDs, but suffers from poor color rendering index. We have investigated Cr and Ce co-doped YAG. Our investigation suggests Cr addition can drastically enrich the emission spectrum of Ce:YAG in the red region, which is realized by a non-radiative energy transfer from the Ce$^{3+}$ 2D$^3/2$ level to Cr$^{3+}$ 4T level. The emission spectrum excited at 467 nm blue wavelength shows that the addition of Cr induces strong peaks in the red region. Comparison with the emission spectrum of the Cr-only sample reveals that the intensity of red Cr emission is much higher in Ce and Cr co-doped samples, which suggests energy transfer from Ce to Cr. Excitation spectra collected at the Cr red emission show a large excitation peak at 458 nm and suggest energy transfer from the 2D$^3/2$ level of Ce$^{3+}$ to the 4T level of Cr$^{3+}$, which is responsible for the enhanced red emission from Cr. At the same time, radiative transfer from Ce$^{3+}$(2D$^3/2$) to Cr$^{3+}$(4T) through the absorption of the yellow emission by Cr seems limited. The orders of magnitude increase in the Cr red emission in Ce/Cr:YAG compared to Cr:YAG suggests that the former is an efficient red and yellow phosphor.
1:51PM B38.00014 Spectral Intensities of Transitions Between Stark Levels of Er$^{3+}$(4f$^{11}$) in Single Crystal, Ceramic, and Nanocrystalline Y$_2$O$_3$, KELLY NASH, JOHN GRUBER, DHIRAJ SARDAR, University of Texas at San Antonio, UYGUN VALIEV, National University of Uzbekistan, NIKOLAI TER-GABRIELYAN, LARRY MERKLE, AROCKIASAMY MICHAEL, Army Research Laboratory — Similarities and differences among the optical properties of Er$^{3+}$Y$_2$O$_3$ in single crystal, polycrystalline (ceramic), and nanocrystalline forms are discussed based on spectra obtained between 400 nm and 1700 nm and temperatures between 8 K and 300K. The observed crystal-field splitting and the measured intensities of transitions between the $^{2S+1}L_J$ manifolds of Er$^{3+}$(4f$^{11}$) in both the C$\alpha$ and C$\beta$ sites are analyzed in terms of models that invoke the mixing of states of opposite parity through the odd terms in the crystal-field Hamiltonian. The inversion symmetry of C$\beta$ sites limits electronic transitions to magnetic dipole transitions between the $^1L_{1/2}$ and $^1L_{5/2}$ manifolds. For Er$^{3+}$ ions in C$\beta$ sites, the forced electric-dipole transitions along with some magnetic dipole contribution in certain cases, are allowed between the J+1/2 Stark levels within all manifolds. Within the instrumental resolution, there are some important differences between intensities of transitions depending on particle size of the Er$^{3+}$Y$_2$O$_3$.

2:03PM B38.00015 Judd-Olfelt analysis and crystal-field modeling of Er$^{3+}$ transitions in YAlO$_3$, SREE R. CHANDRASEKHARAN, University of Texas at San Antonio, KELLY L. NASH, JOHN B. GRUBER, AND DHIRAJ K. SARDAR TEAM — Optical absorption and emission intensities are investigated for trivalent Er$^{3+}$ ions in YAlO$_3$ crystal. The Judd-Olfet model is applied to the room temperature absorption intensities of Er$^{3+}$(4f$^{11}$) transitions in YAlO$_3$ to obtain the intensity parameters which are then used to calculate the spontaneous emission probabilities, branching ratios, radiative decay rates, and radiative lifetimes of the Er$^{3+}$ transitions from the upper multiplet manifolds to the corresponding lower-lying multiplet manifolds in YAlO$_3$. The room-temperature fluorescence lifetimes and the emission cross sections of selected intermanifold transitions are determined. From the calculated radiative lifetimes and the measured fluorescence lifetimes, the quantum efficiency of the sample has been found. The 8K absorption spectrum has been examined as well. Selected manifolds have been analyzed in terms of crystal field splitting using current models and minimization methods to establish the parameters of Er$^{3+}$ in C$_\alpha$ symmetry sites. The optical and spectroscopic characteristics of Er$^{3+}$YAlO$_3$ show that this material has a potential for both 1.5µm and 544.96 nm stimulated emissions.

Monday, March 10, 2008 11:15AM - 2:15PM —
Session B39 GSNP DFD: Focus Session: Collective Dynamics of Self-Driven Particles
Morial Convention Center 231

11:15AM B39.00001 Polar and apolar active matter$^1$, M. CRISTINA MARCHETTI, Syracuse University — Assemblies of interacting self-driven units form a new type of active soft matter with collective behavior qualitatively different from that of its individual constituents, nonequilibrium phase transitions, and unusual mechanical and rheological properties. Examples include cytoskeletal filaments crosslinked by motor proteins, bacterial colonies, migrating cells, and vibrated layers of granular rods. In this talk I will review our work on using nonequilibrium statistical physics to derive a continuum description of these systems from specific models of single particle dynamics. This approach aims at understanding the interplay between physical mechanisms (such as formation or loss of physical connections, excluded volume effects, directional forces) and biochemical or other processes in regulating the large-scale organization and function of active matter. I will contrast the behavior of units with a head and a tail that can exhibit a macroscopic polar state, where all organisms move coherently in a preferred direction, with that of units with head-tail symmetry, that can order in a nematic state, with no net motion on macroscopic scale. Finally, I will use a simple model of active rod on a substrate to discuss the interplay between equilibrium steric effects and self-propulsion in controlling order and fluctuations in active fluids.

$^1$Work done with T. B. Liverpool, A. Ahmadi and A. Baskaran. Supported by DMR-0705105

11:51AM B39.00002 Swarming and swirling in self-propelled polar granular rods, ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA, GEOFFROY LUMAY, GRASP, Physics Department, University of Liège, B-4000 Liège, DMITRI VOLFSON, LEV TSIMRING, Institute for Nonlinear Science, University of California, San Diego, La Jolla, CA 92039 — We discuss the dynamics of “self-propelled” polar rods experimentally and numerically. In the experiment, the polar motion was achieved by vibrating rods with asymmetric mass distribution. In the numerics, we postulate a driving force acting along the axis of the rod. We observe aggregation of rods at the boundaries because of the inability of rods to turn around and escape for high enough density under low noise conditions. As vibration strength and thus noise is increased, the aggregation reduces and a uniformly distributed state displaying local orientation order and swirls are observed. We observe greater than $\sqrt{\pi}$ density fluctuations which are in a qualitative agreement with the Toner-Tu model, but this agreement should not be over-emphasized since the model is directly applicable to a nematic regime. Our findings elucidate an important and interesting interplay between the shape and the directed motion in realistic self-propelled rods which affects the phenomenology of their collective dynamics.

12:03PM B39.00003 Rectification of Swimming Bacteria and Self Driven Particle Systems by Arrays of Asymmetric Barriers, CHARLES REICHHARDT, Los Alamos National Laboratory, Los Alamos NM, MEW BING WANG, Department of Physics, Washington University, St Louis, MO 63160, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory, Los Alamos NM 87545, ZOHAR NUSSINOV, Department of Physics, Washington University, St Louis, MO, 63160 — We show that the recent experimental observation of the rectification of swimming bacteria in a system with an array of asymmetric barriers occurs due to the ballistic component of the bacteria trajectories introduced by the bacterial “motor.” Each bacteria selects a random direction for motion and then moves in this direction for a fixed period of time before randomly changing its orientation and moving in a new direction. In the limit where the bacteria undergo only Brownian motion, rectification by the barriers does not occur. We also examine the effects of steric interactions between the bacteria and observe a clogging effect upon increasing the bacteria density.

12:15PM B39.00004 Delay induced instabilities in self-propelling swimming particles$^1$, ERIC FORGOSTON, IRA SCHWARTZ, Naval Research Laboratory — We consider a general model of self-propelling biological or artificial individuals interacting through a pairwise attractive force in a two-dimensional system in the presence of noise and communication time delay. Previous work has shown that a large enough noise intensity will cause a translating swarm of individuals to transition to a rotating swarm with a stationary center of mass. In this work, we use numerical simulations to show that with the addition of a time delay, the model possesses a transition that depends on the size of the coupling parameter. This transition is independent of the swarm state (traveling or rotating) and is characterized by the alignment of all of the individuals along with a swarm oscillation. By considering the mean field equations without noise, we show that the time delay induced transition is associated with a Hopf bifurcation. The analytical result yields good agreement with numerical computations of the value of the coupling parameter at the Hopf point.

$^1$Research supported by the Office of Naval Research and Army Research Office

12:27PM B39.00005 ABSTRACT WITHDRAWN —
12:39PM B39.00006 From Cannibalism to Active Motion of Groups , PAWEL ROMANZUK, LUTZ SCHIMANSKY-GEIER, Institute of Physics, Humboldt University Berlin — The detailed mechanisms leading to collective dynamics in groups of animals and insect are still poorly understood. A recent study by Simpson et. al. suggests cannibalism as a driving mechanism for coordinated migration of mormon crickets [1]. Based on this result we propose a simple generic model of brownian particles interacting by asymmetric, non-conservative collisions accounting for cannibalistic behavior and the corresponding avoidance strategy. We discuss our model in one and two dimensions and show that a certain type of collisions drives the system out of equilibrium and leads to coordinated active motion of groups.


12:51PM B39.00007 Spatial instability and bioturbulence in highly concentrated bacterial suspensions1 , ANDREY SOKOLOV, IGOR ARANSON, Argonne National Laboratory — We present an experimental study of spatio-temporal organization and transition to complex collective swimming regimes in highly concentrated suspensions of Bacillus subtilis. Experiments are performed in a free-standing thin-film sample with controlled thickness. Novel non-invasive high-resolution optical coherence tomography technique is used to probe the density distributions in the film in real time. Increasing the film thickness beyond certain threshold triggered a transition from quasi-to-dimensional collective swimming to three-dimensional turbulent state which is attributed to Oxygentaxis. We have studied effect of the controlled oxygen concentration on the bacterial collective behavior and transition to turbulent bioconvection.

1This work was supported by U.S. DOE grant DE-AC02-06CH11357

1:03PM B39.00008 Non-Coalescent, Self-Assembling Water Drops: Phase transitions, flows and hydrodynamics , MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, Atlanta GA 30332 — We study the collective nucleation, growth and self-assembly of non-coalescent water drops. These form and organize over evaporating polymer solutions exposed to a draft of moist air. The creation and evolution of a population of drops towards a closed packed array occurs in response to heat and mass fluxes involved in droplet condensation and solvent evaporation. We elucidate the kinetics and dynamics of droplet growth and assembly, by accounting for various transport and thermodynamic processes. These water drops template hexagonally ordered arrays of holes in polymer films. We thus have a useful and economical method for manufacturing porous films requiring only a drop of polymer solution (dilute) and a whiff of breath!

1:15PM B39.00009 Active nematics: fluctuations and coarsening1 , SRIRAM RAMASWAMY, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012, SHRADHA MISHRA, CCMT, Department of Physics, Indian Institute of Science, Bangalore 560 012, INDIA, FRANCESCO GINELLI, HUGUES CHATE, Service de Physique de l’Etat Condense’, CEA/Saclay, 91191 Gif-Sur-Yvette, FRANCE, SANJAY PURI, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, INDIA — Nonequilibrium steady states with spontaneous nematic order are known to arise in collections of amoeboid cells as well as granular-rod monolayers. Recent studies [EPL 62 (2003) 196-202; PRL 96, 180602 (2006); PRL 97 (2006) 012, INDIA, FRANCESCO GINELLI, HUGUES CHATE, Service de Physique de l’Etat Condense’, CEA/Saclay, 91191 Gif-Sur-Yvette, FRANCE, SANJAY PURI, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, INDIA — Nonequilibrium steady states with spontaneous nematic order are known to arise in collections of amoeboid cells as well as granular-rod monolayers. Recent studies [EPL 62 (2003) 196-202; PRL 96, 180602 (2006); PRL 97 (2006) 012, INDIA, FRANCESCO GINELLI, HUGUES CHATE, Service de Physique de l’Etat Condense’, CEA/Saclay, 91191 Gif-Sur-Yvette, FRANCE, SANJAY PURI, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, INDIA — Nonequilibrium steady states with spontaneous nematic order are known to arise in collections of amoeboid cells as well as granular-rod monolayers. Recent studies [EPL 62 (2003) 196-202; PRL 96, 180602 (2006); PRL 97 (2006)

1Supported by CSIR and DST, India

1:27PM B39.00010 Long-range correlations in simulations of suspensions of swimming microorganisms , PATRICK UNDERHILL, University of Wisconsin-Madison, JUAN HERNANDEZ-ORTIZ, Universidad Nacional de Colombia Sede Medellin, MICHAEL GRAHAM, University of Wisconsin-Madison — Simulations of large populations of hydrodynamically interacting swimming particles have been performed at low Reynolds number in periodic and confined geometries. Our simulations show that the interactions of the particles lead to long-range spatial correlations in the fluid at scales larger than the size of a single organism. These long-range correlations lead to a large enhancement in the fluid transport properties. The diffusion coefficient of passive, non-Brownian tracer particles diverges in the periodic geometry with increasing the simulation box size. This collective motion depends on the method the organism uses for propulsion. Simple scaling arguments have also been developed that can capture much of the physics of both the swimmer and tracer motions.

1:39PM B39.00011 Simulated Flocking Dynamics of 2D Self-propelled Hard Particles , DONALD BLAIR, University of Massachusetts Amherst — Following a recent demonstration of long-lived giant number fluctuations in a swarming, granular nematic (Narayan et. al, Science 317, 105 (2007)), we perform 2D simulations of hard, self-propelled particles which communicate only through contact. We vary particle end-shape, polarity, and aspect ratio and explore the effects on order, on the development of density fluctuations, and on the evolution of the swarm boundary. Connections to various forms of active matter (swimming bacteria, crawling cells) will be discussed.

1:51PM B39.00012 Cell swarming leads to vortex flow in early embryo formation , ARIEL BALTER, Biocomplexity Institute, Indiana University, JAMES A. GLAZIER, Biocomplexity Institute, Indiana University — A forming embryo can be thought of as a confined region of incompressible medium. Vortex flow is observed in early embryo formation from drosophila fruit flies to mammals. The Navier-Stokes equation for fluid flow in a cavity is known to have stable vortex solutions. A model for cell motion in which cells move independently of their neighbors corresponds to high Reynolds number (Re) incompressible flow. An alternative cell-swarming model in which cells do influence their neighbors motion (through a mechanism known as contact following) corresponds to a flow model that is similar to low Re incompressible flow. Both models can potentially lead to stable vortex formation in a confined cavity. We investigate the applicability of both models to real biological systems

2:03PM B39.00013 Active elastic dimers: self-propulsion and current reversal on a featureless track , VIJAY KUMAR KRISHNA MURTHY, SRIRAM RAMASWAMY1, CCMT, Dept. of Physics, Indian Institute of Science, Bangalore 560012, MADAN RAO2, Raman Research Institute, Bangalore 560080. — Directed motion without an imposed external gradient is seen not only in living systems but also in agitated granular matter. The essential ingredients are an external energy input and inherent asymmetry. Unlike traditional “Brownian ratchet models”, the asymmetry of interest in the above systems is internal to the motile objects, and does not lie in an external periodic potential. In this work, we present a Brownian inchworm model of a self-propelled elastic dimer in the absence of an external potential. Nonequilibrium noise together with a stretch-dependent damping form the propulsion mechanism. Our model connects three key nonequilibrium features – position-velocity correlations, a nonzero mean internal force, and a drift velocity. Our analytical results, including striking current reversals, compare very well with numerical simulations. The model unifies the propulsion mechanisms of DNA helicases, polar rods on a vibrated surface, crawling keratocytes and Myosin VI. We suggest experimental realizations and tests of the model.

3Supported by CMTU, JNCASR, Bangalore 560064.
4Also at NCBS (TIFR), Bangalore 560065.
11:15 AM B40.00001 Summer 2007: My SPS intern experience and working with ComPADRE\textsuperscript{1}, ANDREW COUGHLIN, Society of Physics Students — For the summer of 2007 I was enrolled in the Society of Physics Students Internship program hosted by the American Institute of Physics in College Park, Maryland. My time at was spent working for the American Physical Society outreach department. My primary task was to expand and maintain Physicstogo.com which is part of the ComPADRE group of outreach websites funded by the National Science Foundation. More specifically, I searched for materials to add to the website, cataloged citation information, and updated the biweekly magazine portion of the website. Work experience was not the only thing gained from this internship. As a group of 8 interns we attended an event on Capitol Hill, met with members of congress, and toured nearly every monument and museum in the area. The 2007 SPS internship was an amazing opportunity and a summer memory that will remain with me for the rest of my life.

\textsuperscript{1}Society of Physics Students

11:27 AM B40.00002 Demonstrating Levitation and Suspension of a Superconductor on a Magnetic Track\textsuperscript{1}, CHARLES P. STREHLOW, M.C. SULLIVAN, Ithaca College — The suspension and levitation of superconductors by permanent magnets is one of the most fascinating consequences of superconductivity, and a wonderful instrument for generating interest in low temperature physics. We present a novel classroom demonstration of the levitation/suspension of a superconductor over a magnetic track that maximizes levitation/suspension time, separation distance between the magnetic track and superconductor as well as insulator aesthetics. A theoretical explanation of the levitation/suspension and a simple mathematical model of the lateral restoring forces are discussed.

\textsuperscript{1}Supported by NSF Grant DMR-0706557.

11:39 AM B40.00003 Comprehensive study on deformation of metal samples based on measurements of temperature, in-plane displacement and stress-strain characteristics , JOHN GAFFNEY, CHRISTOPHER SCHNEIDER, SANICHIRO YOSHIDA, Southeastern Louisiana University — We have studied the dynamics of deformation of metal samples. Our efforts are directed at finding some correlation between the stage of deformation (elastic, plastic, pre-fracturing stage, etc) and changes in properties of the sample such as the change in temperature across the surface, the stress strain characteristics, and the in-plane displacement on the sample surface. To study this, we simultaneously applied three independent data collection systems; a tensile machine to obtain the stress strain curve, an optical interferometer to study both the vertical and horizontal displacement of the surface, and two thermistors to obtain a continuous temperature reading as the sample deformed. With two thermistors, we were able to study how the temperature changed in different locations on the surface of the sample.

11:51 AM B40.00004 Low-temperature calorimeter for magnetocaloric-effect measurements in high magnetic fields , TRAVIS MILLER\textsuperscript{2}, YASUMASA TAKANO, University of Florida — The magnetocaloric effect, in which sweeping a magnetic field results in a temperature variation, is a powerful tool for detecting phase transitions in magnetic samples. The effect is particularly useful near the zero-temperature limit where a transition line becomes horizontal in the field-temperature phase diagram, a temperature region in which specific heat fails to exhibit sharp anomaly at the transition. At temperatures below 200 mK, however, eddy current heating produces a temperature background that becomes relative in magnitude to the temperature change of genuine features, seriously limiting sensitivity. This causes numerous problems in trying to extracting clear data. We describe a new calorimeter design which overcomes this problem in experiments using a dilution refrigerator in magnetic fields up to 20 T.

\textsuperscript{2}Funded by The University Scholars Program at The University of Florida.

12:03PM B40.00005 Driven Intrinsic Localized Modes in a Coupled Pendulum Array, RITOBAN BASU THAKUR, Dickinson College, LARS ENGLISH, ALBERT SIEVERS, Cornell University, DICKINSON COLLEGE, PHYSICS TEAM — Intrinsic localized modes (ILMs), also called discrete breathers, are directly generated via modulational instability in an array of coupled pendulums. These ILMs can be stabilized over a range of driver frequencies and amplitudes. They are characterized by a \( \pi \) -phase difference between their center and wings. At higher driver frequencies, these ILMs are observed to disintegrate via a pulsating instability, and the mechanism of this breather instability is investigated.

12:15PM B40.00006 Quartz tuning fork as a viscometer for Helium liquids\textsuperscript{1}, J. JHAVERI, M. GONZALEZ, P. BHUPATHI, Y. LEE, Department of Physics, University of Florida, Gainesville, FL 32611-8440 — Oscillating beams serve as simple systems for measuring effects of energy dissipation as a result of interaction with their environment. Especially in miniature mechanical oscillators, the enhanced surface-to-volume ratio signifies the importance of damping caused by drag force. We have investigated the mechanical response of commercial miniature quartz tuning forks with a natural resonant frequency of 32.768 kHz. The changes in resonance frequency and damping have been measured at various Helium and Nitrogen gas pressures and various temperatures. Our results will be compared with theoretical predictions in order to extend its application to the sub-millikelvin temperature range as an effective thermometer in superfluid \( ^3 \)He.

\textsuperscript{1}This work is supported by NSF grant no. DMR-039483 and University Scholars Fellowship at University of Florida (J.J).

12:27PM B40.00007 Demonstrating the Principle of an rf Paul Ion Trap, ANDREW JOHNSON, JAMES RABCHUK, Western Illinois University — An rf ion trap uses a time-varying electric field to trap charged ions. This is useful in applications related to quantum computing and mass spectroscopy. There are several mechanical devices described in the literature which have attempted to provide illustrative demonstrations of the principle of rf ion traps, including a mechanically-rotating “saddle trap” and the vertically-driven, inverted pendulum\textsuperscript{1,2}. Neither demonstration, however, successfully demonstrates BOTH the sinusoidal variation in the electric potential of the rf trap AND the parametric stability of the ions in the trap described by Mathieu’s equation. We have modified a design of a one-dimensional ponderomotive trap\textsuperscript{3} so that it satisfies both criteria for demonstrating the principle of an rf Paul trap. Our studies indicate that trapping stability is highly sensitive to fluctuations in the driving frequency. Results from the demonstration apparatus constructed by the authors will be presented.\textsuperscript{1} Rueckner, W., et al., “Rotating saddle Paul trap.” Am. J. Phys., 63 (2), February 1995. \textsuperscript{2} Friedman, M.H., et al., “The inverted pendulum: A mechanical analogue of a quadrupole mass filter,” Am. J. Phys., 50 (10), October 1982. \textsuperscript{3} Johnson, A.K. and Rabchuk, J.A., “A One-Dimensional Ponderomotive Trap,” ISAAPT 2007 spring meeting, WIU, March 30, 2007.
12:39PM B40.00008 Experimental characterization of piezoelectric THUNDER actuator shape, PAUL HARRIS — A new type of piezoelectric composite actuator called THUNDER, which was originally developed by NASA, has potential applications in micro robotics, aeronautics, acoustics and hydraulics. The manufacturing process produces internal stresses with accompanying structural deformation. It is the aim of this research to characterize these deformations. Detailed measurements were taken by a motion control LabView data acquisition system and measured with a laser micrometer on several different types of actuators. Several functional forms were used in an attempt to fit the data. The data was best fit by a circular segment function. We also used a transcendental equation to be able to compare to other single point published values. We found the range of dome heights to be between 10.15 mm and 1.45 mm. For one particular model, the manufacturing difference was found to be 16% with an experimental error of 0.5%. The robust experimental data is vital to the development of our finite elements models. Preliminary experimental results of voltage induced deformations will be presented.

12:51PM B40.00009 A Relativistic Understanding of Rotating Reference Frames, KACEY MEAKER, TOM MICHALIK, Randolph College (founded as Randolph-Macon Woman’s College) — The purpose of this research is to obtain a greater understanding of relativistic acceleration and rotation. Particles in a rod experiencing constant acceleration have hyperbolic worldlines. A simple global rigid rotating frame cannot be physically realized, because the force needed to maintain an object in circular motion approaches infinity. This understanding will be discussed in this presentation.

2:00PM Session CI APS: Poster Session I: 2:00 pm - 5:00 pm Morial Convention Center Exhibit Hall A

C1.00001 POLYMERIC AND ORGANIC MATERIALS I —

C1.00002 Molecular Dynamics of Polymer Systems on Graphic Processing Units (GPUs)¹, JOSHUA ANDERSON, Iowa State University and Ames Laboratory, CHRIS LORENZ, Kings College London, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Molecular dynamics (MD) is a powerful, but computationally intensive, simulation technique capable of modeling a wide range of systems in and out of thermodynamic equilibrium. Using traditional computers, simulations large enough to explore the phases of polymer systems require the use of expensive distributed memory clusters. Graphics Processing Units now offer an unprecedented amount of computing power for general purpose applications. They are inexpensive ($500) and can be added to almost any standard desktop system. MD algorithms are adapted to execute on a single GPU, which is able to attain the same performance as 32 processor cores on a cluster. It is possible for a single system to host up to 4 GPUs, putting the power of a 128 processor core cluster on the desktop. This performance is illustrated in a variety of polymer systems such as low density micellar phases with cubic symmetry, high density lamellar and nanocomposite gyroid systems. GPUs offer unprecedented opportunities for the simulation of polymer systems.

¹This work is supported under NSF grant DMR-0426597 and DOE contract no DE-AC02-07CH11358

C1.00003 An Efficient Algorithm to Calculate Density of State in Large Systems: Generalized Ensemble Means and Compression-Variable Transformation¹, XIN ZHOU, T7, Los Alamos National Laboratory — We present a high efficient algorithm to calculate density of state (DOS, or its logarithm, \( S(U) \)) of large systems in any macroscopic variable \( U \). The algorithm calculate the ensemble means and fluctuations of \( U \) in a series of generalized ensembles to form \( S(U) \) and its derivative in some adaptively generated \( U \), then interpolate whole the \( S(U) \) curve within the required accuracy. We also apply a compression transformation in the \( U \) space to focus the most computation cost on extrapolating \( S(U) \) in new \( U \) region. The algorithm is found to be order of \( O(N^{1/2}) \) (or faster) as the increasing system size \( N \), which is far faster than all current available methods (at least \( O(N^{3/2}) \)). The algorithm satisfies the detailed-balance condition in whole simulations by averaging the ensemble means in each segment of simulation by using their errors as weight, so that it has great numerical stability. The method can be combined with the parallel tempering (PT) algorithm to simulate the low-temperature properties of large complex fluids and decrease the number of the needed replica in original PT, \( O(N^{1/2}) \), to one in each macroscopic phase. The validity of the new approaches are demonstrated by presenting the simulated results of Lennard-Jone liquids with different size \( N \). The approaches even generate DOS of each super-saturated macroscopic phase in the unstable liquid/solid coexistence region, respectively, which provides much more information to understand the phase coexistence and transitions.

¹This work was supported by the US DOE under contract No. DE-AC52-06NA25396.

C1.00004 Understanding Thermodynamics and Surface Dynamics of Pom-pom Branched Polystyrene, SEWOO YANG, The University of Akron, DAVID T. WU, Colorado School of Mines, ZHANG JIANG, SURESH NARAYANAN, Argonne National Laboratory, MARK D. FOSTER, The University of Akron — We have studied the effect of varying the relative length of the central linear portion of the pom-pom chain on the size of a single chain and on the bulk thermodynamics of blends of the pom-pom branched polystyrenes (PS) with linear analogs. A novel set of pom-pom PS with well-defined molecular architecture was synthesized anionically. The value of the interaction parameter contribution of the bulk chains and both the scattering of a single pattern analyzed and time correlation performed to obtain correlation functions. The temperature dependence for the \( q \)-dependent relaxation time was determined and estimates of the surface tensions of the different polymers derived from the static structure factors.

C1.00005 Synthesis and characterization of erbium (III)-doped polyimide nanofibers for low temperature thermophotovoltaic applications¹, ZHENXIN ZHONG, DARRELL RENEKER, Dept of polymer science, University of Akron — Thermophotovoltaic conversion technology is a promising way to convert waste heat to electricity via photons. In this research, erbium (III)-doped polyimide nanofiber mats were prepared as selective emitters to explore the selective thermal emission efficiency in a low operating temperature range (< 500 °C). The selective emission at 6500 cm\(^{-1}\) of erbium (III)-doped polyimide nanofiber mats was measured on mats characterized with scanning electron microscopy, transmission electron microscopy, FT-IR spectroscopy, and thermogravimetric analysis. A small but potentially useful amount of power was obtained from a 2 mg mat.

¹We acknowledge the financial support from NSF grant # DMI-0403855.
Characterization of an electrospinning jet from videographic observations of glints

KAIYI LIU, CAMDEN ERTLEY, DARRELL RENEKER, Dept. of Polymer Sci., The Univ. of Akron — Detailed relationships between glints of light reflected from the electrical bending coils of an electrospinning jet and the path of the jet were established. The path of the jet was observed by illuminating the jet with a short, intense flash of light. Glints were formed simultaneously by a continuous, intense beam of light from a chosen set of directions. As the jet path moved through the continuous beam of light, some segments of the path were oriented so that intense specular reflection (a glint) was recorded by a camera. The motion of the jet path caused a glint to create a trace in the videographic image. A linear glint trace divided into two traces when the segment producing the glint became involved in a bending instability. A smooth turn of a coil of the jet path usually produced two glints in a particular observation direction. When the smooth turn became involved in a smaller electrical bending coil, the two glints divided into many glints. Observations of this sort are expected to lead to new ways to reduce the variability in the diameter of electrosyn polymer nanofibers.

We acknowledge financial support from the National Science Foundation, DMI-0600733.

Viscoelastic Electrospinning Jets: Initial Stresses and Elongational Rheometry

HAN, Dept. of Polymer Science, U of Akron, ALEXANDER YARIN, Dept of Mechanical and Industrial Engineering, U of Illinois at Chicago, DARRELL RENEKER, Dept of Polymer Science, U of Akron — A novel method of characterization of longitudinal stresses in electrospinning jets is introduced. The measured initial longitudinal stresses in jets of a 6 wt% aqueous solution of polyethylene oxide (Mn = 400 kDa) were of the order of 100 kPa, which is two orders of magnitude larger than in other free viscoelastic jets. This is attributed to strong stretching of polymeric liquids in the transition zone between the Taylor cone and the beginning of the jet, where the stretching rates are 100 to 1000 s⁻¹. The velocity of the fluid along the straight segment was determined from the observed jet diameter combined with the laser Doppler velocimeter data. The tensile stress was measured by creating a lateral displacement, near the beginning of the jet, and observing its propagation along the jet. Combination of the velocity with the stress data provided the information needed to determine the modulus and relaxation time of a polymeric liquid subjected to rapid stretching.

We acknowledge the financial support from NSF grant # DMI-0600733.

Molecular Modeling of Thermosetting Polymers

SOUMYA PATNAIK, Air Force Research Laboratory, VIKAS VARSHNE, Universal Technology Corporation, BARRY FARMER, Air Force Research Laboratory — In this work we present molecular modeling of thermosetting polymers with special emphasis on building atomistic models. Different approaches to building highly cross-linked polymer networks starting from un-crosslinked systems are discussed. A multi-step procedure for relaxing the molecular topology during crosslinking was proposed which allows for minimizing the increase in the residual internal stresses with increasing degree of crosslinking. This methodology was applied to epoxy based thermosets and several materials properties such as density, Young’s modulus, glass transition temperature, thermal expansion coefficient and volume shrinkage during curing were calculated and found to be in good agreement with experimental results. Along with the materials properties, the simulations also highlighted the distribution of molecular weight build up and inception of gel point during the network formation.

Nafion/poly(1-vinyl imidazole) composite membranes for fuel cell application

DUKJOON KIM, Sungkyunkwan University, SUNGYUNKWAN UNIVERSITY TEAM — A base monomer (1-vinyl imidazole, VIdz) was polymerized in Nafion® 112 membrane by UV irradiation in order to reduce methanol permeability of the latter. With increasing content of poly 1-vinyl imidazole (PVI), equilibrium water uptake was decreased due to reduced size of hydrated ion cluster in the composite membrane as confirmed by a small angle X-ray scattering analysis. The electrochemical properties of the membrane such as ion conductivity, methanol permeability and electro-osmotic drag were also affected by equilibrium water uptake and hydrated pore size. Even a minute incorporation of the base polymer showed a significant effect on proton conductivity and methanol permeability. Methanol transport by electro-osmotic drag was evaluated by using relating equations and methanol permeability and limiting current density data obtained in this study. Although the absolute number of electro-osmotic drag was hard to determine, the trend of change could be studied in relation to bulk-like water in composite membranes. This novel composite membrane exhibited an increased cell performance compared with a plain Nafion membrane due to reduced methanol crossover rate.

Metastable Structures of poly(lactic acid)

JEFF KALISH, SHAW L. HSU, University of Massachusetts Amherst, KAORU AOU, Dow Chemicals, MEG STARKWEATHER, University of Massachusetts Amherst — The coexistence of two poly(lactic acid) crystals (alpha and alpha’) and its impact on the double melting peaks in differential scanning calorimetry is investigated. Solubility differences as well as irreversibility of the alpha to alpha’ transformation process indicates that the alpha’ crystal is the less stable crystal form. The difference in thermal stability is quantified by measurement of crystal melting enthalpies using the Pyda/Wunderlich method. The relative composition of the crystalline fraction can also be determined by the same method. Crystal annealing is found to be accompanied by an increase in both overall crystallinity and the fraction of the alpha crystal relative to the alpha’ crystal. Infrared spectroscopy is used to probe the crystal structures. In comparison to the alpha crystal, the alpha’ crystal is found to have a weakened carbonyl-carbonyl intermolecular interaction. Results also suggest that the alpha’ crystal does not have a 10/3 helix which constitutes the alpha crystal. The coexistence of the two crystal forms has profound implications in interpretation of double melting peaks in its DSC thermogram.

Perturbing Effects of Bulky Comonomers on the Chain Conformation of Poly(vinylidene fluoride)

SURYIYAKALA RAMALINGAM, YUNING YANG, SHAW L. HSU, University of Massachusetts Amherst — The comonomer effect on structures of poly(vinylidene fluoride- hexafluoropropylene) copolymers (PVDF-HFP) was analyzed by Raman spectroscopy. The HFP content of these copolymers varies from 5% to 15%. Because of steric interactions involving the bulky HFP comonomers, the predominant chain conformation has extensively more gauche conformers in comparison to pure PVDF. Based on both experimental and simulation studies, specific spectroscopic features in the 700 cm⁻¹ region have been identified that are characteristic of irregular chain conformations elucidating the perturbing effect of HFP on the equilibrium chain statistics of PVDF in the amorphous phase. In addition, these spectroscopic features were revealed to be extremely sensitive to the relative placement of CF₃ units respective to other fluorine atoms along the chain.

Single Crystals of Diblock Copolymers: Tethered Chain Study

RYAN M. VAN HORN, JOSEPH X. ZHENG, HUIMING XIONG, RODERIC P. QUIRK, University of Akron, BERNARD LOTZ, Institut Charles Saudron, EDWIN L. THOMAS, Massachusetts Institute of Technology, STEPHEN Z.D. CHENG, University of Akron — Tethered polymer chains have become an important area of research over the last few decades. Their unique properties make them appealing for various applications. The tethering density of the chains is the most important parameter in determining their properties, as shown by various theoretical and experimental works. Our group uses single crystals of crystalline-amorphous diblock copolymers to study tethered polymer chains. This system provides better control of tethering density and molecular weight as compared to previous methods. Previous work on PS-b-PEO and PS-b-PLLA shows, for the first time, the values of the interacting and brush regime transitions. The systems studied have addressed some issues, molecular weight dependence and solvent quality, but they do not provide general results. The work presented here will look at the role of chain adsorption and crystallization of the tethered chain, using PMMA-b-PLLA and PEO-b-PCL systems.
C1.00013 Morphological Control of Segmented Polyurethanes via Crystallization Confinement of Soft Segments, MATTHEW HOOD, BINGBING WANG, JOHN LASCALA, JAMES SANDS, FREDRICK BEYER, JOSH ORLUCKI, MARK VANLANDINGHAM, CHRISTOPHER Y. LI, U.S. ARL COLLABORATION — Segmented polyurethane (SPU) is a linear, high molecular weight block copolymer comprised of regions of soft and hard segments. The phase separation between these mechanic-contrasting segments is partly the cause of SPU’s superior mechanical strength as the hard domains reinforce the soft domains, while the soft domains provide the toughness that allow for good energy adsorption. To achieve the greatest impact absorption the soft segments must remain amorphous surrounding the crystallized hard domains which are held together via hydrogen bonding. We systematically investigated a SPU system with poly(ethylene glycol) (PEG) of various molecular weights as the soft segments. Using differential scanning calorimetry, small angle X-ray scattering and wide angle X-ray diffraction it was observed that as hard segment content increased there was a decrease in soft segment crystallization till PEG crystallization was no longer observed, thus achieving the desired structure. By tailoring the composition it is also possible to control the nano-sized structure altering the morphology on the macro-scale thus increasing the interface density of the SPU such that we produce a transparent film possessing structural capabilities suitable for transparent body armor.

C1.00014 Crystal Size Effect on Dielectric Property of PVDF at High Electric Field and Its Effect on Energy Storage and Discharging Behaviors, FANGXIAO GUAN, STEVEN BOGGS, LEI ZHU, Institute of Material Science and Department of Chemical, Materials and Bimolecular Engineering, University of Connecticut, Storrs, CT 06269-3136 — Improvement of the high energy density capacitor can be achieved by choosing a material with relatively high dielectric constant and/or high electric breakdown strength. In general, their relationship can be described as $E_0 R_0^2$. For certain dielectric polymers, such as poly (vinylidene fluoride) (PVDF), dielectric constant shows strong electric field dependence. Therefore, the energy density cannot be described simply by this equation. In this work, electric field dependent dielectric response of PVDF is studied, and its relation to the energy density stored is discussed. Although the dielectric constants of PVDF with different crystal sizes can be different at high electric field, they all have similar stored energy density. Intriguingly, their energy discharging behaviors are different. The smaller the crystal size, the faster the energy discharging process, and the lower the dielectric loss. From this study, we conclude that a high energy density with fast discharge and low dielectric loss could be obtained by tuning the crystal sizes.

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C1.00015 Reducing Dielectric Loss by PVDF-CTFE Graft Copolymers, JING WANG, ZHONGZHE YUAN, FANGXIAO GUAN, STEVEN BOGGS, LEI ZHU, Institute of Material Science and Department of Chemical, Materials and Bimolecular Engineering, University of Connecticut, Storrs, CT 06269-3136 — Polymer film capacitors with high energy density and low loss are very attractive in potential applications. Maintaining the high dielectric breakdown strength in high dielectric constant films with a low loss will also be a challenge. Poly(vinylidene fluoride) (PVDF) and its copolymers are well-known ferroelectric polymers that exhibit excellent electromechanical properties as candidates for high-performance, high-energy-density capacitor. However, the dielectric loss of commercially extruded PVDF films is high (0.02). In our work, lower dielectric loss polystyrene (PS) were introduced to improve PVDF dielectric properties. PVDF-CTFE-g-PS graft copolymers were synthesized via the “graft from” process. The quality of films from graft polymer was improved, resulting high energy density and low loss. A series of graft polymers with different electric properties were prepared, since the breakdown strength and dielectric loss of PVDF were influenced by the crystallinitities and crystal sizes.

This work was supported by ONR Grant N00014-05-1-0338.

C1.00016 Semicrystalline Polymers: A special case of polymer brushes, VIKRAM KUPPA, GREGORY RUTLEDGE, Massachusetts Institute of Technology — Monte Carlo (MC) molecular simulations are employed to evaluate the interface between crystalline and amorphous polyethylene. The simulation setup mimics the interlamellar region of a semicrystalline polymer with a low effective molecular weight. All polymer chains are tethered to the crystal surface at one of their ends, thus forming tails with their other (free) ends distributed in the space between crystal lamellae. Two different systems are explored: one, in which the simulations explore a range of molecular weights due to the use of MC moves that exchange beads between different chains; and another, in which strict control of the molecular weight is exercised, thereby constraining chain lengths to a narrow window. The effects of temperature, grafting density, molecular weight distribution and the interaction between brushes on opposing crystal surfaces are investigated by examining monomer density profiles, chemical potentials and bond orientation order parameters.

C1.00017 Polydomain Simulation of Liquid Crystalline Polymer Orientation in Channel Flows, JUN FANG, WESLEY BURGHARDT, Northwestern University — The properties of liquid crystalline polymers are strongly affected by the molecular orientation state induced by processing flows. LCP structure development under flow is quite complex, due to the propensity towards ‘director tumbling’ dynamics in rodlike nematics, and the resulting complicated ‘polydomain’ distributions of orientation. Many models of LCP structure & rheology begin with a detailed description of the molecular orientation state, possibly including a molecular description of distortional elasticity. While well suited for simulations of fundamental phenomena in simple flows, application of these models to processing flows is far out of reach. Conversely, the phenomenological polydomain model of Larson & Doi is sufficiently simple to allow for its application to process simulations. This is further facilitated by a nearly exact analogy between the Larson-Doi model and the Folger-Tucker model for predicting orientation in fiber dispersions, which is incorporated in commercial process simulation software. We use this available modeling infrastructure to test the ability of the Larson-Doi model to predict orientation distributions in kinetically complex but isothermal channel flows of liquid crystalline polymers, comparing simulation results orientation distribution data previously obtained using in situ x-ray scattering methods.

C1.00018 Thin Film morphologies of rod-coil block copolymers, MANAS SHAH, VENKAT GANESAN, University of Texas at Austin — The interplay of microphase separation and liquid crystalline ordering in rod-coil block copolymers leads to complex morphologies distinct from that of conventional flexible block copolymer phases. For many electronic and semi-conducting applications, rod-coil block copolymers need to be patterned into thin films. The final morphology and the nature of orientation of rod units would now depend (in addition to the constituent interactions) on the interactions of the blocks with the confining surfaces. We combine the self-consistent field theory models of rod-coil block copolymers in a thin film framework to understand the effect of confinement on the morphology and the nature of orientation of rod-units.

C1.00019 Structural Recovery of Epoxy Films Subjected to CO$_2$ Pressure Jumps, SHANKAR KOLLENGODU-SUBRAMANIAN, Texas Tech University, MATAZ ALcoutlabi, University of Utah, LAMECK BANDA, The Dow Chemical Company, GREGORY MCKENNA, Texas Tech University — This group has previously investigated the impact of structural recovery and physical aging on thermodynamic and mechanical properties of polymers after temperature jumps and compared with plasticizer jumps [1]. Increasing plasticizer content depresses the glass transition temperature ($T_g$) in glassy polymers and this results in changes in the mechanical, optical and dielectric properties. Plasticizer jumps using a strong polar molecule have been previously studied by our group and have shown qualitatively similar behavior to temperature jump experiments [2]. In the current work, we report the results on plasticization effects using a weakly polar molecule (CO$_2$) on the structural recovery of glassy polymers after plasticization jumps and compare the behavior with temperature formed glasses.


C1.00020 Strain induced non-linear effects in Dynamic Viscosity measurements1. J.P. IBAR, IPREM University of Pau, 64013 Cedex — Melt viscosity measurements conducted at increasing \( \omega \) and strain, in a parallel plate dynamic rheometer, trigger a roaster of non-linear effects which we review, such as variation from the commanded strain, non-linearity between stress and strain, time dependence of the G' and G" moduli, and appearance of slip. In addition, melt fracture, at the surface or in the bulk has been reported. Both the Torque and the Normal Force are studied. Results from both a constant strain rheometer (RDAII) and a constant stress rheometer (Bohlin SVO are reviewed. We examine the many aspects of non-linearity and explore the origin(s) of these manifestations, whether due to measurement limitations, melt instability, or purely the expression of non-linear viscoelasticity.

1 Under Fulbright Grant

C1.00021 Topology of Branched Polymers: Effect on Structure and Dynamic Properties1. RAMNATH RAMACHANDRAN, GREGORY BEAUCAGE, AMIT S. KULKARNI, University of Cincinnati, VASSILIOS GALIATSAOS, DOUGLAS C. MC-FADDIN, LyndellBasell Industries — We investigated linear and branched polyethylene (PE) using small-angle neutron scattering (SANS). The experiments were conducted on dilute solutions of PE in deuterated p-xylene. A variety of structural information1 such as fractal dimension \( d_f \), connectivity dimension \( c \), minimum path dimension \( d(min) \), long chain branch fraction \( \phi_b \), radius of gyration \( R_g \) and persistence length \( l_p \) were obtained. Such information presents a qualitative and quantitative assessment of branching in polymers. Theoretical models such as ‘binary contacts per pervaded volume’ model were employed to correlate the structural information of the polymer to its entanglement molecular weight \( (M_e) \). \( M_e \) was used to predict physical properties of the polymer such as plateau modulus \( (G'_{\infty}) \) and zero-shear viscosity \( (\eta_0) \). 

C1.00022 Entanglement Percolation Effects on the Dynamics of Polymer Rheology. RICHARD WOOL, Department of Chemical Engineering, University of Delaware — The percolation model of entanglements (Wool 1983) makes unique predictions regarding the dynamics of polymer chains, in the terminal relaxation zone of reptating linear polymer melts of molecular weight M. When percolation occurs during relaxation of entangled chains in the terminal zone, we observe some unusual results. These include: (a) for homopolymers of molecular weight \( M >> M_e \), reptating chains appear to be non-reptating as their ends and centers relax at the same rate during percolation. (b) During stress relaxation, the random coil dimensions \( R_g(\perp) \) and \( R_g(\parallel) \) are predictably not fully relaxed when the stress and birefringence relax to zero. (c) The matrix molecular weight \( P \) effects on relaxation time \( \tau \) of the probe chain \( M >> M_e \) are as follows: Rouse-like dynamics is observed for reptating chains with \( \tau \sim PM^2 \) when \( M >> P \) and (d) the relaxation time \( \tau \sim P^{-3}M^2 \) when \( P >> M \), in accord with reptation. These unusual results predicted by entanglement percolation are supported by significant experimental data from selectively deuterated polystyrene chains HDH, DHD and DPS. Entanglement Percolation replaces Constraint release and Chain End Fluctuation mechanisms in the understanding of the dynamics of polymers in the melt and concentrated solutions.

C1.00023 Determining Local Mechanical Properties of Soft Materials with Cavitation Rheology. JESSICA ZIMBERLIN, NAOMI SANABRIA-DELONG, GREGORY TEW, ALFRED CROSBY, University of Massachusetts — To guide the development of tissue scaffolds and the characterization of naturally heterogeneous biological tissues, we have developed a method to determine the local modulus at an arbitrary point within a soft material. The method involves growing a spherical cavity at the tip of a syringe needle and monitoring the pressure of the cavity at the onset of a mechanical instability. This critical pressure is directly related to the local modulus of the material. Using model hydrogel, materials, we demonstrate the ability for this technique to quantify the local stiffness of hydrogel networks and its relation to the macroscopic stiffness as measured by shear rheometry. In addition to heterogeneities in equilibrium hydrogel networks, we quantify differences in local stiffness during the gelation of hydrogels. Lastly, we consider the influence of surface energy on the onset of cavitation by using different injected agents to induce the instability.

1 Authors would like to acknowledge NSF-IGERT and NSF-MRSEC for their support.

C1.00024 Caviation Rheology of Polyacrylamide Hydrogels. SANTANU KUNDU, JESSICA ZIMBERLIN, ALFRED CROSBY1, University of Massachusetts-Amherst — Cavitation rheology is a new characterization technique for the measurement of mechanical properties on small length scales, e.g. 10 -100 \( \mu \)m, at any arbitrary location within a soft material. The technique involves growing a cavity at the tip of a syringe needle and monitoring the pressure of the cavity at the onset of instability. This critical pressure is directly related to the local modulus of the material. We used this technique to characterize the network mechanics of polyacrylamide hydrogel materials, a common material used in many biological applications. We applied the cavitation rheology results with that obtained from shear rheometry. This technique was used to investigate the rheological properties of gels with different dimensions and different moduli, which were obtained by varying initial monomer to water ratio. These results provide a quantitative foundation for the extension of this technique to in vivo characterization of biological tissues.

1 corresponding author

C1.00025 Polyurea segmented multi-block copolymers: structure and dynamics. JAI PATHAK, JEFFREY TWIGG, C. M. ROLAND, PETER MOTT, NRL, Chemistry, DEREK HO, ERIC LIN, NIST, Polymers, MARY VUKMIR, THOMAS EPPS, JAI PATHAK, University of Delaware, Chemical Engineering — We study a Polyurea copolymer by measuring its stress-strain behavior between 100 and 1000 inv. s strain rate and by oscillatory shear rheology, respectively. Polyurea shows elastomeric mechanical response over a wide temperature range, as the rigid domains physically cross-link the soft domains. The modulus increases, while the residual strain in samples stretched to failure decreases with increasing strain rate. SAXS on undeformed specimens reveals two peaks: a higher wave-vector peak from semi-crystalline hard segments (long period 6 nm), and a lower wave-vector peak from micro-phase separated domains of spacing 70 nm. Polyurea specimens quasi-statically stretched to failure show anisotropic scattering, suggesting that deformation effects on morphology are controlled by rigid domain response over the deformation time-scale. Greater molecular reorganization and alignment take place at low strain rates. At large strain rates no molecular reorganization is possible, yielding identical structure as undeformed materials, pronounced strain-rate hardening and low residual strain.
C1.00026 Nanoscale Superstructures in Copolymers with Evenly Spaced Charged Groups.

WENQIN WANG, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6272. SHARLENE R. WILLIAMS, TIMOTHY E. LONG, Department of Chemistry, Virginia Tech, Blacksburg, VA 24061-0334. RALPH H. COLBY, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802-5007. KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6272. — Multiple copolymers with evenly spaced charged groups have been synthesized: poly(ethylene-PE)-based ionenes, poly(tetramethylene oxide)-PTMO)-based ionenes, and poly(alkylene oxide)-based sulfonated polyester ionomers. The morphologies of these copolymers are investigated using differential scanning calorimetry, X-ray scattering, and electron microscopy. In both PE- and PTMO-based ionenes, the bulky cationic groups in the backbone reduce the crystallinity of the copolymer and form cation-rich channels perpendicular to the polymer backbone, where the extent of association is influenced by the size of the ionic liquid moiety. In the sulfonated polyester ionomers, the crystallization of long poly(alkylene oxide) segments promotes the formation of ion-rich layers. These results will be compared with our recent work with linear poly(ethylene-co-acrylic acid) copolymers and ionomers with precisely spaced acid groups.

C1.00027 Phase behavior of polyelectrolyte multilayers investigated by thin film calorimetry.

H. HUTH, University Rostock, Institute of Physics, Uniplatz 3, 18051 Rostock, Germany. R. MUELLER, MPI fuer Kolloid-und Grenzflaechenforschung, Am Muelchenberg, 14424 Potsdam, A. FERY, University Bayreuth Physical chemistry II, Universitaetsstr. 30, 95447 Bayreuth, C. SCHICK — Polyelectrolyte multilayer can be easily assembled using spraying or dipping of the different polyelectrolytes [1]. The thickness of the produced layers (nanometer range) is well controlled by the preparation conditions. Only few methods are available for dynamic investigations, as afo for mechanical properties [2]. AC-chip calorimetry is used as a very sensitive tool for calorimetric investigations of such thin films as demonstrated for thin polymeric films [3]. To investigate the phase behavior of polyelectrolytes the humidity is used as a new parameter in addition to temperature for calorimetry. First measurements with the modified calorimeter for the PSS/PDADMAC polyelectrolyte multilayer system are shown. Further extensions of the calorimeter for better understanding of the phase behavior are discussed.

C1.00028 Stimulus-Response of Charged Diblock Copolymer Brushes.

DONG MENG, QIANG WANG, Colorado State University. — We have performed self-consistent field calculations to study the stimulus-response of diblock copolymer brushes on a planar substrate. One of the two blocks carries either weakly or strongly dissociating charges, making the brush surface responsive to the solution pH, ionic strength and applied electric field, in addition to the solvent selectivity. We have investigated in detail the influence of these stimuli on the polymer segmental distribution and surface switchability of the brush. Our result can be used to guide the experimental design of “smart surfaces” from diblock copolymer brushes.

C1.00029 Characterization of polyelectrolyte behavior of the polysaccharides chitosan, heparin, and hyaluronan, by light scattering and viscometry.

SOHEIL BODDI, SUSAN YONEMURA, MATT KIPPER, Colorado State University. — This study on the polyelectrolyte behavior of polysaccharides in solution is motivated by our recent work in development of nanostructured polysaccharide-based surface coatings. Chitosan behaves as a weak polyanion, and hyaluronan behaves as a weak polyanion, while heparin behaves as a strong polyanion. The ability to control the conformation of these polysaccharides in solution, by changing the solution ionic strength and pH may offer the opportunity to further tune the nanoscale features of polysaccharide-based surface coatings assembled from solution. In the work reported here, the solution conformation of these polymers is determined from gel permeation chromatography coupled to differential refractive index, light scattering, and viscometry detection. These results are related to the nanostructure of chitosan-heparin and chitosan-hyaluronan surface coatings based on polyelectrolyte multilayers.

C1.00030 Competition between liquid crystalline (LC) ordering and block copolymer (BCP) microphase separation in a series of LCBCPs.

KISHORE TENNETI, Drexel University, XIAOFANG CHEN, Peking University, CHRISTOPHER LI, Drexel University, XINHUA WAN, QI-FENG ZHOU, Peking University, LIXIA RONG, BENJAMIN HSIAO, Stony Brook University, DREXEL UNIVERSITY TEAM, PEKING UNIVERSITY COLLABORATION, STONY BROOK UNIVERSITY COLLABORATION — A comprehensive study displaying a rich variety of liquid crystalline (LC) phase structures (SmA, ColN, ColH, ColR) and block copolymer (BCP) morphologies (tetrangular perforated and transverse-parallel lamellae) observed in liquid crystalline LCBCP systems will be presented. The systems under investigation differ in the flexibility of interactions between the mesogen and polymer backbone. Both non-covalent and covalent interactions are investigated in a series of mesogen-jacketed-, side-chain- and hydrogen bonded- LCBCPs and the influence of composition and molecular architecture on the final phase behavior will be presented. The factors that lead to the domination of either LC ordering or BCP microphase separation will also be reported.

C1.00031 Symmetry transition in multilayer films of block copolymer/homopolymer blends.

VINDHYA MISHRA, E.J. KRAMER, UCSB — Multilayer films of spherical domain poly(styrene-b-2vinyl pyridine) (PS-PVP Mn:65000, f_pvp = .12) blended with 5 vols % low molecular weight PS homopolymer (Mn:13000) is characterized with grazing-incidence small angle x-ray diffraction (GISAXD) to determine the lattice symmetry and stacking of layers. The structure was also imaged by transmission electron microscopy (TEM). In such films competition between packing preferred at the surfaces with that preferred by the internal layers leads to a transition in the packing symmetry as n, the number of sphere layers, increases. Pure PS-PVP exhibits hexagonal close packed (HCP) symmetry up through n=4. At n=n* =5 the in-plane symmetry becomes face centered orthorhombic whose lattice parameters approach those of the BCC (110) plane for n>>10. GISAXD and TEM data from the blend films one to ten layers thick shows that the addition of 5 vol % PS increases n* to 7. We think that the PS segregates to the interstices in the HCP structure reducing the stretching of the PS blocks and the free energy penalty of HCP versus BCC inner layers. Significant improvement in translational order is also seen in all the films over the copolymer alone.

1GISAXD experiments conducted at Advanced Photon Source, Argonne National Laboratory

C1.00032 Hierarchical Assemblies of Block Copolymer-Based Supramolecules in Thin Films.

SHIH-HUANG TUNG, NISHA C. KALARICKAL, THOMAS SCHILLING, TING XU, Department of Materials Science and Engineering, University of California at Berkeley — Diblock copolymer-based supramolecules can be constructed by associating small molecules to the side chain of one block. In bulk, supramolecules self-assemble into a rich library of hierarchical structures. However, the phase behaviors of such systems in thin films have been rarely studied. Here, we present a structural investigation of polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) with hydrogen-bonded 3-pentadecylphenol (PDP) to P4VP block in thin films. We show that using the same diblock copolymer, a variety of hierarchical structures can be obtained by varying the stoichiometry of P4VP to PDP. More importantly, the lamellar and cylindrical microdomains can be oriented normally to the substrates after annealed under chloroform atmosphere. The assembly of P4VP/PDP complex, ca. 4nm in size, is oriented within the microdomain as confirmed by GISAXS and AFM. Thus, control over the supramolecular assemblies at two length scales, i.e. tens of nanometers and a few nanometers, can be simultaneously achieved in thin films.

3We acknowledge APS for facilitating the GISAXS experiments performed as part of this work.
C1.00033 Solvent annealing of block copolymer thin films combined with controlled dewetting

TAE HEE KIM, CHEOLMIN PARK, Yonsei University — The treatment of block copolymer thin film with its solvent vapor has been known as an effective way to control both orientation of microdomains with respect to the surface and their registration into a well defined periodic lattice structure. We have recently demonstrated hierarchically ordered cylindrical microdomains in a poly(styrene-b-ethylene oxide) (PS-b-PEO) thin film combined with microcontact printing. Well ordered PEO microdomains in large area was successfully produced by confined dewetting of thin PS-b-PEO films micropatterned on chemically modified surfaces with self-assembled monolayers during solvent annealing. In order to further control block copolymer thin films upon solvent annealing, we introduce a new patterning method of block copolymer thin films, Plasma Enhanced Polymer Transfer Printing (PEPTP) where a block copolymer thin film spin cast directly on a patterned PDMS mold is easily transferred to a substrate with oxygen plasma. The microstructure of the block copolymer film micropatterned by PEPTP is ordered by the subsequent solvent annealing. The controlled microstructures were characterized by Atomic Force Microscope (AFM), Field Emission Scanning Electron Microscope (FESEM) and Grazing-Incidence Small Angle X-ray Scattering (GISAXS).

C1.00034 Morphological Study of ABC Triblock Terpolymers

SATOSHI AKASAKA, AKIKO MITANI, HIROKAZU HASEGAWA, Department of Polymer Chemistry, Kyoto University, NIKOS HADJICHRISTIDIS, Department of Chemistry, University of Athens — Triblock terpolymers form richer variety of microdomain structures than diblock copolymers. In this study We investigated the microdomain structures in the toluene-cast films of several kinds of ABC triblock terpolymers consisting of polystyrene, polyisoprene and poly(dimethyl siloxane) (PS-b-PI-b-PDMS) by transmission electron microscopy (TEM). As the result we observed various structures composed of lamellae, cylinders and spheres. In addition, we employed electron tomography to analyze the two complex network-forming structures using their three-dimensional images. Consequently, we found that one of them forms core-shell type double gyroid structure in PS matrix, and the other forms core-shell type single gyroid-like structure in PS matrix.

C1.00035 Stimuli-responsive block copolymers in ionic liquids

TAKESHI UEKI, University of Minnesota, MASAYOSHI WATANABE, Yokohama National University, TIM LODGE, University of Minnesota, YOKOHAMA NATIONAL UNIVERSITY COLLABORATION — Ionic liquids (ILs) are room temperature molten salts and have attracted much attention because of their unique properties. The characteristics of ILs (non-volatility, non-flammability, chemical stability, high ionic conductivity) can contribute to high performance energy-conversion materials. On the other hand, some polymers greatly change their solubility in ILs in response to external stimuli such as temperature and light. We have found that poly(N-isopropylacrylamide) (PNIPAm) and poly(benzyl methacrylate) (PBnMA) show upper critical solution temperature (UCST)-type phase behavior and lower critical solution temperature (LCST)-type phase behavior in an ILs, respectively. Most recently, we also discovered that certain polymers change their solubility induced by photo stimuli. In this study, we describe temperature and photo stimuli responsive self-assembly of AB type block copolymers having at least one stimuli-responsive segment in IL solution. Based on the results, we will apply to construct stimuli-responsive physical gels by using ABA triblock copolymer self assembly in an IL.

C1.00036 Polymer translocation through a nanopore in presence of attractive binding particles

ANIKET BHATTACHARYA, University of Central Florida, KAIFU LUO, TAPIO ALA-NISSILA, Helsinki University of Technology, SEE-CHEN YING, Brown University — We use Brownian dynamics simulation to study the translocation of a flexible linear polymer chain through a nanopore into a cell containing particles those bind reversibly to the chain. We study the role of these binding particles [1] by monitoring the mean first passage time, the diffusion of the center of mass, and the net force on the translocating chain as a function of the density of these particles and the strength of the attractive interaction.


C1.00037 Thin Film Morphology of Block Copolymers Containing Polydimethylsiloxane as a Function of the Surface Tension of the Opposing Block

Maurice Wadeley, kevin cavicchi, Dept. of Polymer Engineering The University of Akron — The self-assembly of block copolymers into ordered nanostructures such as spheres, cylinders, and lamellae in the range of 10-100 nm makes them interesting materials for patterning surfaces. Thin films of block copolymers containing poly(dimethylsiloxane) (PDMS) are attractive for patterning due to their high oxygen etch resistance compared to other polymers. The main disadvantage of these polymers for patterning is the low surface tension of PDMS. This causes the preferential migration of PDMS to the air/film interface driving the formation of domains parallel to the interface and surface wetting layers. In this work a series of AB block copolymers containing PDMS have been prepared where the surface tension of the opposing block was varied. The effect of changing the surface tension mismatch between the blocks on the thin film morphology will be discussed.

C1.00038 Novel diblock copolymer morphologies under cylindrical confinement

PRIYANKA DOBRIYAL, THOMAS P. RUSSELL, University of Massachusetts, Amherst — Cylinder forming polystyrene-b-polystyrene diblock copolymers were introduced inside nanoparticles of alumina membrane. The pore diameter was varied in order to study the effect of confinement on diblock copolymer morphologies. The molecular weights of the polymers were also varied and similar morphologies were obtained for similar degree of confinement. The morphologies observed were dependent on the structural frustration (D/Lo), where D is the pore diameter and Lo is equilibrium period spacing. D/Lo was varied from 0.75 to 2. A rich variety of novel morphologies that include single helix, toroids and double helices were observed which are not observed in the bulk. These morphologies also depended upon the surface of the pore walls. Different morphologies were obtained when the pore wall was neutral for same structural confinement.

C1.00039 Hard-Surface Effects in Diblock Copolymer Systems

DONG MENG, YUHUA YIN, JACQUELINE ACRES, QIANG WANG, Colorado State University — Polymer chains near a hard (impenetrable) surface have different conformations from those in the bulk. For diblock copolymers (DBC), a hard surface has both energetic and entropic effects. The decrease of polymer segmental density near a hard surface reduces A-B repulsion and favors self-assembled morphologies with more B-A interfaces near the surface, while the enrichment of chain ends and depletion of middle segments near the surface favor parallel morphologies where chains orient mainly perpendicular to the surface. Using parallel self-consistent field calculations with high accuracy, we have studied in detail the hard-surface effects in three DBC systems: DBC thin films confined between two flat homogeneous surfaces, DBC in nanopores, and DBC nanocomposites.

C1.00040 Structural Rearrangement of Miscible Polymer Blends at the Polymer/Substrate Interface

XIGUO ZENG, SHAH L. HSU, University of Massachusetts Amherst, BRIGITTE WANG, CHARLES W. PAUL, National Starch & Chemical — Structural rearrangement of miscible polymer blends upon contact with a hard substrate has been investigated using Raman Micro-spectroscopy. In this study, blends of crystallizable poly(hexamethylene adipate) (PHEMA) and acrylic random copolymer resin were observed on substrates of polycarbonate (PC), polypropylene (PP), and polymethyl methacrylate (PMMA). Results showed distinct selective migration and subsequent adsorption of polymer at the polymer/substrate interface. The final compositional distribution at the interface is determined by the type of substrate. Theoretical calculations based upon the Flory-Huggins theory were carried out relating the interaction parameter (chi) and miscibility of polymer blends and different substrates. The combined experimental and theoretical results clearly demonstrate that specific interactions at the interface are primary causes for structural rearrangement. Furthermore, the chain mobility and molecular weight of polymer blends were also found to be important factors affecting the migrations and consequent surface adsorption ratios.
C1.00041 A Deuterium NMR Study of Water in a Blend of Soy and Polyether Polyols , VUE ZHAO, XIA TONG, SHAW L. HSU, University of Massachusetts Amherst — The reaction of water with disocyanate is crucial in formation of polyurethane foams. It yields polyurea hard segments whose lengths and segregation from the polyether soft segments depends, among other things, on the reaction kinetics largely determined by the miscibility of water in the polyether. For soy polyol-based polyurethane formulations, the miscibility issue is further complicated by the use of hydrophobic soy polyols. The question of where water molecules are located in the multicomponent blend is of importance; the answer is key to understanding how the morphology and phase separation evolve and are correlated with foam performance. With water content typically around 5%, it has long been challenging to find a technique that can provide this critical information. We developed an NMR method based on the use of deuterium oxide and found that the signal of resonance of deuterium is sensitive to the chemical environment, which allows water molecules to be quantitatively traced in the phase-separated blend of soy and polyether polyols. Moreover, the resonance signal could serve as a probe to monitor the evolution of phase separation upon composition and temperature change.

C1.00042 Surface segregation of end-functionalized homopolymers in a homopolymer matrix , MICHAEL DIMITRIOU, CRAIG HAWKER, EDWARD KRAMER, UCSB — Surface segregation of end-functional poly(2-vinylpyridine) in a blend with P2VP was measured by X-ray photoelectron spectroscopy. A series of chain end functionalized P2VP homopolymers were synthesized via either anionic polymerization or Reversible Addition Fragmentation Chain Transfer RAFT and end capped with either a single fluorinated oligomer or a perfluorinated dendrimer. The degree of end functionalization was characterized using NMR spectroscopy, IR spectroscopy and gel permeation chromatography (GPC).

C1.00043 Identification of self consistent field interaction parameter from continuum Monte Carlo simulation of model polymer blends , JUN KYUNG CHUNG, DAVID MORSE, University of Minnesota — Monte Carlo simulations of binary AB polymer blends have been performed to evaluate the effective interaction parameter \( \chi \) of self consistent field theory, and to quantify corrections to RPA predictions for fluctuations. We consider a model with a non-bonded pair interaction \( v_{ij}(r) = v_{1}(r) \) for which \( f(r) = \) the repulsive Lennard-Jones form, \( \epsilon_{AA} = \epsilon_{BB} \), and \( \epsilon_{AB} = \epsilon_{AA} + \Delta \epsilon \). Using thermodynamic perturbation theory, to first order in \( \Delta \epsilon \), we obtain an interaction free energy with the composition dependence predicted by Flory-Huggins theory, with an effective interaction parameter \( \chi_{e} = \chi_{e} \). Here, \( z_{e} \) is an effective coordination number given by the average of the sum of values of \( f(r) \) for interactions between a test monomer and nearby monomers on other chains, in a reference system with \( \Delta \epsilon = 0 \). Results for composition fluctuations in semigrand ensemble simulations of blends with a range of values of \( \Delta \epsilon \neq 0 \), for several chain lengths, are compared to RPA predictions calculated using this perturbatively defined \( \chi_{e} \) parameter.

C1.00044 Theory For The Miscibility Windows In Blends Of Polypropylene And Ethylene-\( \omega \)-Olefin Copolymers , DAVID WU, HUIMIN LI, Colorado School of Mines, JOHN CURRO, University of New Mexico, COLORADO SCHOOL OF MINES COLLABORATION, UNIVERSITY OF NEW MEXICO COLLABORATION — The miscibility of isotactic polypropylene (iPP) and ethylene-and \( \omega \)-olefin (C2Cs) copolymers has been intensively studied both for its industrial importance and as a model system for complex polymer miscibility behavior. Experiments generally show a window of miscibility in particular regions in the parameter space defined by copolymer composition, volume fraction, and branch chain length. Since the cost of systematic molecular dynamics studies of such systems is still prohibitive, a statistical mechanical approach with the molecular interaction potentials and chain structure as the only input is highly desirable. We present self-consistent Polymer Reference Interaction Site Model (SC-FRISM) calculations for blends of iPP and C2Cs copolymer, where \( C_{x} \) is propylene, butene, and hexene. The calculated enthalpy of mixing is shown to correlate well with experimental trends for the miscibility window. Furthermore, since the theory allows access to molecular-level correlations, insight is provided into the mechanisms for the specific miscibility behavior, including contributions due to chain conformations.

C1.00045 MALDI-ToF Analysis of Model Copolymer Blends , DAVID PAN, MARK ARNOULD, Xerox Corporation — MALDI-ToF mass spectrometry was used to determine the composition of a low MW styrene (S) / n-butyl acrylate (nBA) copolymer. Bernoullian chain statistics were used to predict the copolymer distribution and confirm that MALDI-ToF detects the correct composition. The copolymer was blended with a low MW polystyrene homopolymer having the same end group as the copolymer at several levels to determine if MALDI-ToF could be used to calculate the amount of homopolymer by subtracting the iPP and C2Cs copolymer peaks, where \( C_{x} \) is propylene, butene, and hexene. The calculated enthalpy of mixing is shown to correlate well with the experimental trends for the miscibility window. A model to improve the accuracy of the calculated amount of homopolymer in the blend is discussed.

C1.00046 Tuning the morphology of polymer nanocomposites: Effect of film thickness and nanoparticle shape1,2, SANGAH GAM, AYESNUR CORLU, RUSSELL J. COMPOSTO, University of Pennsylvania — Adding nanoparticles (NPs) to polymer blend films is an attractive route towards enhancing the mechanical, optical, and electronic properties. Previously, we showed that NPs can segregate to the interphase, jam and produce stable bicontinuous structures. In this study, we show how film thickness effects the phase behavior of poly(methyl methacrylate): poly(styrene-ran-acrylonitrile) (PMMA:SAN) blends containing PMMA-modified silica NPs that partition to the PMMA/SAN interface. As NP loading increased and film thickness decreased, the growth of PMMA domains and correlation length was slowed down. As film thickness increased, the critical concentration to achieve jamming decreased suggesting that lower loading can be used to create bicontinuous structures. To investigate NP shape, hydroxyl and methyl-modified silica nanorods (NRs) were added to PMMA:SAN films. These NRs partitioned into the PMMA-rich domains and produced smaller domain size with increased loading. Compared to spherical NPs, NR loading was more effective at slowing down phase evolution.

C1.00047 Synthesis and Characterization of Polyamide Nanocomposites Using Functionalized Carbon Nanotubes , MOHAMMAD MONIRUZZAMAN, KAREN WINEY, University of Pennsylvania, JAYANTA CHATTOPADHYAY, W. EDWARD BILLUPS, Rice University — We have synthesized nylon 6,10 nanocomposites using functionalized single-walled carbon nanotubes using our interfacial \textit{in situ} polycondensation method. The specific functional groups \(- (C_{2}H_{4})_{n}COCI \) on the sidewalls of SWNT were designed to covalently link the nanotubes to the nylon matrix via alkyl segments. The composites show significant improvements in tensile modulus, strength and toughness. The alkyl linkages at the SWNT/nylon 6,10 interface contribute significantly to improving the toughness of the composites. Two extensions of this work will be presented. First, our method will be altered to synthesize nylon 6 via ring opening polymerization in the presence of functionalized nanocomposites. Second, we will adapt our method to other functionalized nanoparticles, possibly graphite. We expect to achieve similar improvements in mechanical properties in these composites.

C1.00048 Bulk and Thin film Properties of Nanoparticle-based Ionic Materials , JASON FANG, MSE CORNELL UNIVERSITY, ITHACA, NY TEAM — Nanoparticle-based ionic materials (NIMS) offer exciting opportunities for research at the forefront of science and engineering. NIMS are hybrid particles comprised of a charged oligomeric corona attached to hard, inorganic nanoparticle cores. Because of their hybrid nature, physical properties — rheological, optical, electrical, thermal — of NIMS can be tailored over an unusually wide range by varying geometric and chemical characteristics of the core and canopy and thermodynamic variables such as temperature and volume fraction. On one end of the spectrum are materials with a high core content, which display properties similar to crystalline solids, stiff waxes, and gels. At the opposite extreme are systems that spontaneously form particle-based fluids characterized by transport properties remarkably similar to simple liquids. In this poster I will present our efforts to synthesize NIMS and discuss their bulk and surface properties. In particular I will discuss our work on preparing smart surfaces using NIMS.
C1.00049 Natural Rubber - Layered Silicates Nanocomposites: Mechanical Properties, Structure & Dynamics. HARIS RETSSOS, MSE CORNELL UNIVERSITY, ITHACA, NY TEAM, IPST-CSIC, MADRID, SPAIN TEAM — Natural Rubber (NR) is one of the most industrially relevant elastomers due to unique elastic properties. Recently we have been developed NR composites with incorporated natural or synthetic clays. We present structural, dynamical and mechanical properties to justify the influence of different parameters, like silicate dispersion, cross-linking density and strength of polymer/silicate interface, on the reinforcement phenomena of those composites. To understand the improvement of the mechanical properties we have investigated the possibility of any bound rubber formation on the outer surface of fillers like in carbon black or silica composites. Evidence from a rather similar situation have been found in silicate nanocomposites by dielectric spectroscopy and the existence of a possible relaxation mode suggests a strong adhesion with the fillers (interfacially adsorbed polymer IA) that corresponds to a glass transition around 100 °C higher than the bulk glass transition.

C1.00050 Multilayered Polymeric Photonic Structure for THz applications. CHEN XIA, LOUIS KOSNOSKY, JIE SHAN, Physics Department, Case Western Reserve University, JOSEPH LOTT, MATTHEW MACKEY, VISHVAS PETHE, ERIC BAER, ANNE HILTNER, CHRISTOPH WEDER, Department of macromolecular science and engineering, Case western Reserve University — Photonic crystal have been widely studied in the visible, and recently become of interest in the THz regime of the electromagnetic spectrum. We have developed a rapid, easy and cost effective method for the preparation of polymeric materials with high refractive indices (RI) for the terahertz (THz) frequencies through extrusion of polymer and nanoparticles of inorganic materials. Using this method, we have fabricated a one-dimensional photonic crystal of polymer/polymer ferroelectric nanoparticles composite with a nearly complete stop band in the THz regime. The result will also be compared to a transfer-matrix calculation.

C1.00051 Controlled Transdermal Iontophoresis by Polypyrrole/Poly(Acrylic Acid) Hydrogel. PHITHUPHA CHANSAI, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — Transdermal drug delivery system delivers a drug into a body at desired site and rate. The conductive polymer-hydrogel blend between polypyrrole (PPy) doped with anion drug and poly(acrylic acid) (PAA) were developed as a matrix/carrier of drug for the transdermal drug delivery system that characteristic releases depend on the electrical field applied. The PAA films and their blend films were prepared by solution casting using ethylene glycol dimethacrylate (EGDMA) as a crosslinking agent. A mechanical blending of PPy particles and PAA matrix was then carried out. Drug diffusions in the blended PPy/PAA hydrogel and the non-blended one were investigated and determined by using a modified Franz-diffusion cell with an acetate buffer, pH 5.5, at 37 °C, for a period of 48 hours to determine the effects of crosslinking ratio and electric field strength. Amounts of the released drug were measured by UV-Visible spectrophotometry. The diffusion coefficient of drug was determined through the Higuchi equation via different conditions, with and without an electric field. Moreover, thermal properties and electrical conductivity of the polypyrrole and drug-loaded polypyrrole were investigated by means of the thermogravimetric analysis and by using a two-point probe meter, respectively.

C1.00052 Development of PEDOT-PSS/Zeolite Composites as a Gas Sensor. POJJAWAN CHANTHAANONT, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — Polymer-based gas sensors have received considerable interest in recent years, due to the gas sensing ability through the electrical conductivity changes when exposed to a particular gas. In our work, poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonic acid), PEDOT-PSS, was synthesized via an oxidative polymerization and zeolites were used as selective microporous adsorbent to improve selectivity and electrical conductivity sensitivity of the sensors. PEDOT-PSS were fabricated with zeolites by dry mixing and compressed to form PEDOT-PSS/zeolite composites. Zeolite ZSM-5 of various Si/Al mole ratios were chosen. The composites of zeolite ZSM-5 with different Si/Al mole ratios were investigated for the effect of Si/Al mole ratio on the electrical conductivity sensitivity response when exposed to CO and H2.

C1.00053 Effect of Elastomers Types to the Dielectrophoresis Force and Electromechanical Responses. RUKSAPONG KUNANURAKSAPONG, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — Electroactive polymers have been well known as materials for using in many applications such as actuators, MEMS devices, and artificial muscles. In our work, we investigated the effect of elastomers type on the dielectrophoresis force and the electromechanical responses at various electric field strengths. The specimens were prepared by solvent casting method and cut into thin films. We studied the dielectrophoresis forces of all elastomers by measuring the deflection distance under various electric field strengths (0-600 V/mm), and calculated the force from non-linear deflection theory of cantilever. Our data show that the electromechanical responses and the dielectrophoresis forces of all elastomers increase almost linearly with increasing electric field strength. The acrylic elastomers (AR71) has the lowest electrical yield point (75 V/mm) and it generates the highest force (389 µN at E = 600 V/mm). On the other hand, AR70 had the highest electrical yield point (300 V/mm) and it generates the lowest force (321 µN at E = 600 V/mm). The dielectrophoresis forces appear to depend on several factors such as dielectricity, electrical conductivity, and the storage modulus of elastomers.

C1.00054 Development of poly(ether ether ketone)(PEEK) derived from bisphenol-S for proton exchange membrane (PEM) in direct methanol fuel cells (DMFC). SAIRUNG CHANGKHAMCHOM, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — The currently used Proton Exchange Membrane (PEM) in Direct Methanol Fuel Cell (DMFC) is Nafion®, an excellent proton conductivity in fully hydrated membrane. However, it has major drawbacks such as very high cost, and lost of conductivity at elevated temperature and low humidity. In our work, the novel PEM was based on sulfonated poly(ether ether ketone) (S-PEEK) which was synthesized by the nucleophilic aromatic substitution polycondensation of bisphenol-S, 4,4’-dichlorobenzophenone (DCBP), and sodium 5,5’-carbonylbis(2-chlorobenzenesulfonate) (SDCBP). Bisphenol-S is expected to improve thermal stability due to its high melting point (245°C). S-PEEK was characterized by FTIR, 1H-NMR, TGA, DSC, and titration to determine the degree of sulfonation (D.S.). Composite membranes were prepared by using S-PEEK as polymer matrix and heteropolyacid (HPA) as an inorganic filler. The phosphotungstic acid (PTA) was used due to its highly proton conductivity at high temperature and low water uptake. The membranes were characterized by SEM, TGA, DSC, DMA, and by the measurements of the water uptake (%), the swelling ratio (%), the ion exchange capacities (IEC), the melinum diffusion coefficient, and the proton conductivity.

C1.00055 The Titanium-Boron Nitride interaction. GERARDO J. VAZQUEZ, FERNANDO MAGANA, EDUARDO RANGEL, GREGORIO RUIZ, Instituto de Fisica — The Boron Nitride (BN) has a structure very similar to that of graphite and this what makes it interesting to study. A sheet of BN has a structure similar to that of the graphene. In this work it was studied, using molecular dynamics based on pseudopotentials theory and Density Functional Theory (DFT), the energy of interaction of a titanium atom with a sheet of BN to obtain the position of adsorption of the titanium in this system.
BULENT AKGUN, NIST Center for Neutron Research/ Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, SUSHIL SATJIA, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, HOSUB KIM, KOOKEON CHAR, School of Chemical Engineering and Institute of Chemical Process, Seoul National University, Seoul 151-744, Korea — Surface structure and swelling behavior of polyelectrolyte multilayer films of poly(allylamine hydrochloride) (PAH)/poly(sodium 4-styrenesulfonate) (PSS)/poly(methacrylic acid) (PMAA) have been studied using X-ray and neutron reflectivity (NR). Samples have been prepared either using spin-assisted self assembly or dip coating. Swelling measurements were done in a chamber by using saturated salt solutions. PSS/PMAA blend composition was varied from pure PSS to pure PMAA. We experiment the effect of strong polyelectrolyte on the swelling of the multilayer film. Multilayer films prepared by spin assisted deposition yields well defined films with much smooth interfaces than the films prepared by dip coating. NR results showed that incorporation of strong polyelectrolyte, PSS, into the multilayer decreases the swelling capacity of the film.

C1.00057 Drop retention force as a function of drop size, AISHA LEH, RAFAEL TADMOR, PREETI YADAV, PRASHANT BAHADUR, KUMUD CHAURASIA, LAN DANG, Lamar University — In literature, the force, f, required to slide a drop on a surface is often considered as linear with the width of the drop, w, so that f/w is constant. Dussan’s equation further simplifies this proportionality in the case of advancing and receding contact angles constant with drop size, to show that f/V^{1/3} is constant; V being the drop volume. We show experimentally, however, that f/V^{1/3} is usually a decaying function of V. The Dussan equation shows that the change of f/V^{1/3} with V is also expressed in contact angle variation. Our results, however, illustrate that contact angle variation within the scatter suffices to explain the force variation. It becomes easier to predict contact angle variation based on force variation than vice versa. f/V^{1/3} appeared to decrease more with V in the systems studied.

C1.00058 Comparison of AFM and Density Functional Theory Force Profiles, KEENAN DOTSON, JOHN MCCOY, DANIEL MCCOY, Materials Department, New Mexico Tech, Socorro, NM 87801, SERGIO MENDEZ, JOHN CURRO, BRETT ANDRZEJEWSKI, GABRIEL LOPEZ, DAVID KELLER, Chemical and Nuclear Engineering Department, Univ. of New Mexico, Albuquerque, NM 87131 — Monolayer films of tethered poly(N-isopropylacrylamide) in water (and related systems) are investigated with Atomic Force Microscopy. The resulting profiles are analyzed with Density Functional Theory. Of interest are the effects of temperature, degree of polymerization, and surface coverage upon the colloidal force. A particular challenge is the modeling of the adhesive behavior of the film to the coated AFM tip.

C1.00059 Influence of Molecular Weight and Processing Conditions on the Thermal Stability of Nanoimprinted Polymer Structures, YIFU DING, HYUNWOOK DING, KYLE ALVINE, BRIAN OKERBERG, National Institute of Standards and Technology, JING ZHOU, JACK DOUGLAS, ALAMGIR KARIM, CHRISTOPHER SOLES, National Institute of Standards and Technology — We study the influence of both molecular weight of a polymer resist and the nanoimprint process conditions on the thermal stability of the patterned polymer structures. Specifically, we measure the decay rate of the imprinted polymer patterns during thermal annealing by combining diffraction/reflectance of X-ray light and AFM. As a result, highly entangled polymers are found to contain large amount of residual stresses introduced by the imprinting process, which dominates the pattern decay during the annealing. Levels of the residual stresses can be controlled by the imprinting conditions. On the contrast, unentangled polymers behave like a Newtonian liquid with no sign of residual stress resulted from the patterning process. Furthermore, we also observe correlated lateral pattern instability during the annealing, in addition to the vertical pattern decay. This lateral instability is greatly enhanced when the surfactants were added during the imprint process. Implications of these findings on the nanoimprint fabrication processes will be discussed.

C1.00060 Transitions in Nanometer thin films - Investigations by AC Chip calorimetry, H. HUTH, A. MINAKOV, C. SCHICK, University Rostock, Institute of Physics, Uniplatz 3, 18051 Rostock, Germany — Calorimetry is known as a very powerful tool for the characterization of a wide variety of materials and their transitions. The combination of silicon technology and calorimetry opens up new possibilities in this research area as demonstrated recently. Based on a differential AC calorimeter we show an improved experimental setup combining the advantages of the different methods. The measurements are done at slow scanning or at constant bath temperature. The frequency chosen provides a well defined time scale of the experiment. In several cases, e.g. at glass transition, a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible. Due to the differential setup we achieve a sensitive in the pico Joule per Kelvin range allowing to measure samples below one nanogram and consequently films down to 1 nm thickness. Because of the small total heat capacity (addenda + sample) not only a high sensitivity is achieved but AC measurements at relative high frequencies are possible too.

C1.00061 Adhesion of Surface Ribbons, CHELSEA DAVIS, ALFRED J. CROSBY, University of Massachusetts Amherst — Inspired by numerous examples in nature, significant research advances have recently demonstrated the ability to use topographic surface patterns to control critical surface properties such as adhesion and friction. Although most efforts have focused on the use of lithographically-fabricated fibribular structures, alternative patterns such as surface wrinkles have also been shown to be advantageous for the control of adhesion. We present a new surface structure for soft, elastomeric materials called surface ribbons. These surface structure shells are formed by the controlled buckling of a surface-attached film, and offer many advantages for the control of adhesion, including on-command responsiveness. We present methods for the fabrication of these structures, results demonstrating the ability for these structures to enhance adhesion, and scaling relationships that link the structures’ geometry, materials properties, and measured surface properties. In addition to providing attractive avenues for the creation of responsive surfaces, these structures offer fundamental insight into the mechanisms controlling general patterned surface adhesion.

C1.00062 Analysis of the spincoating of thickness gradient polymer films, MONIKA MICHALEK, JOHN DUTCHER, University of Guelp — Thickness polymer films can be prepared by dropping one drop of a polymer solution onto a spinning substrate at a position that is displaced from the axis of rotation, resulting in films in which the thickness increases with increasing radial distance. We have studied the spincoating of polystyrene thickness gradient films in two ways: (1) by fitting the measured radial thickness profiles of the dry films to a simple analytical model; and (2) by measuring the drying of the films during the spincoating process by monitoring the time dependence of the intensity of laser light reflected from the film. The results obtained for solutions of polystyrene dissolved in solvents of different volatility will be compared.

C1.00063 Segmental dynamics of thin polymer films probed by dye reorientation, KEEWOOK PAENG, HAU-NAN LEE, STEPHEN SWALLEN, MARK EDIGER, Department of Chemistry, University of Wisconsin-Madison — We have studied the dynamics of both freestanding and supported polymer thin films (down to 25 nm) by probing reorientation of dilute dye molecules. Well below Tg, dye molecules were photobleached using intense linearly polarized light creating an anisotropic distribution. Anisotropy was measured using circularly polarized light and probing fluorescence parallel and perpendicular to the bleaching beam. Temperature was linearly ramped during anisotropy measurement; near Tg, the anisotropy dropped to zero. The dynamics of a 50 nm poly (tert-butyl styrene) film were faster than bulk dynamics by an amount equivalent to a 5 K shift in Tg. Faster dynamics compared to bulk films were also found for polystyrene and these results will be compared to the previous Tg measurements. Four different polymers, polystyrene, poly (tert-butyl styrene), poly (methyl methacrylate), and poly (2-vinyl pyridine) were studied.
C1.00064 Drop retention force as a function of rested time . RAFAEL TADMOR, AISHA LEH, KUMUD CHAURASIA, PRASHANT BAHADUR, LAN DANG — The force, f, required to slide a drop past a surface is shown to be a growing function of the time, t, the drop waited resting on the surface prior to the commencement of sliding along it. In this first report on the “rest time” effect we demonstrate the existence of this phenomenon in different systems, which suggests that this phenomenon is general. We show that df/dt is never negative. The shorter the resting times, the higher df/dt is. As the resting time increases df/dt decreases towards zero (plateau) as t tends to infinity. We attribute this phenomenon to the corragation of the surface by the drop due to the unsatisfied normal component of the Young equation.

C1.00065 Controlled Growth of Organic Semiconductor Films Using Liquid Crystal Solvents . KEVIN BUFKIN, BROOKS OHLSON, BEN HILLMAN, BRAD JOHNSON, DAVID PATRICK — Interest in using organic semiconductors in applications such as liquid crystal displays, photovoltaic devices, and RFID tags stems in part from their prospects for enabling significantly reduced manufacturing costs compared to traditional inorganic semiconductors. However, many of the best performing prototype devices produced so far have involved expensive or time-consuming fabrication methods, such as the use of single crystals or thin films deposited under high vacuum conditions. It presents a new approach for growing low molecular weight organic crystalline films at ambient conditions based on a vapor-liquid-solid growth mechanism using thermotropic nematic liquid crystal (LC) solvents. Tetracene is deposited via atmospheric-pressure sublimation onto substrates coated by a LC layer oriented using rubbing polyimide, producing films that are highly crystalline, with large grain sizes, and possessing macroscopic uniaxial orientation. This poster will describe the growth mechanism, discuss the effects of processing conditions such as LC layer thickness, substrate temperature and flux rate, and compare the results to a model of diffusion limited aggregation accounting for the finite thickness of the solvent layer.

C1.00066 Single-chain conformation and dynamics in connected chambers: Theory and simulation of translocation and threading . ERICA SALTZMAN, CHIUTAI ANDREW WONG, MURUGAPPAN MUTHUKUMAR, University of Massachusetts at Amherst — Confinement in a series of small chambers connected by narrow pores may be viewed as a model system for translocation in the absence of an applied force, as well as for more general instances of spatially heterogeneous confinement relevant to biological and materials applications. Brownian dynamics simulations are performed for single chains equilibrated in this system, and a theoretical treatment is developed. Short chains undergo translocation between chambers, while long chains thread several chambers and diffuse more rapidly. Measures of chain size and mobility are analyzed and compared.

C1.00067 Monte Carlo simulations of the selective adsorption of heteropolymers on heterogeneous surfaces . YONGMEI WANG, JESSE ZIEBARTH, University of Memphis — Lattice Monte Carlo simulations are used to study selective adsorption of heteropolymers on heterogeneous surfaces. We focus on how statistical correlation between sequence types and surface patterns affects the critical adsorption point (CAP). We show that statistically patchy and statistically alternating surfaces selectively adsorb blocky and alternating chains, respectively, while surfaces with a random distribution of attractive sites do not selectively adsorb any types of chains. We also show that selectivity is maximized near the CAP. Selectivity of checker-board surfaces have also been examined and we show that higher order parameters describing sequences and surface patterns are needed to fully characterize the selectivity of these surfaces toward different sequences.

C1.00068 Progress on a ‘spectral filtering’ for SCFT algorithms: Removing topological defects in block copolymer simulations . SCOTT SIDES, Tech-X Research Corporation, BOBBY SUMPTER, Oak Ridge National Labs — Using block copolymers as mesoscale templates has potential applications for improved photovoltaic devices, fuel-cells and magnetic storage media. For many of these applications the long-range order and orientation of the copolymer phase-separated domains is crucial. Self-consistent field theory (SCFT) for dense polymer melts has been highly successful in describing complex morphologies in block copolymers. Field-theoretic simulations based on SCFT theory are able to access large length and time scales that are difficult or impossible for particle-based simulations such as molecular dynamics. It has been shown that real-space numerical SCFT calculations can describe certain features of topological defects in a bulk copolymer. However, for large SCFT simulations the presence of these topological defects can obscure the identification of the appropriate lowest-energy space group for a complex block copolymer mixture. A ‘spectral filtering’ algorithm has been shown to help reduce the presence of topological defects in SCFT calculations of block copolymer structure by removing certain frequency components of the chemical potential fields during the simulation. Further progress on this filtering method will be presented and shown to improve the removal of defects in large, 3D-SCFT simulations.

C1.00069 Computer simulation of the formation of random-blocky copolymers . LAWRENCE STRICKLAND, JAN GENZER, CAROL HALL, North Carolina State University — A recent computational study described a new method for producing random copolymers (RCPs) with tunable monomer sequence distribution; the technique is based on adjusting the size of a homopolymer (say A) coil and performing a chemical reaction (“coloring”) with certain chemical mienities (say B) on the accessible monomers of the homopolymer chain. While experimental evidence exists that can relate the comonomer distribution in the A-B copolymer to the original homopolymer dimension in the solvent, the “coloring” mechanism is difficult to reconcile as there exists competing mechanisms, involving the coloring process itself and the tendency for the copolymer to change conformation during the “coloring” driven by the changing solubility of the resultant A-B copolymer relative to that of the A homopolymer. In this work we use discontinuous molecular dynamics (DMD) to comprehend the formation of A-B copolymers. Our RCPs were constructed by reacting homopolymers in varying solvents and reagent concentrations. We show how we can selectively tune the randomness by varying chain length and system temperature. While increasing system temperature leads to formation of A-B copolymers with random distribution of segments, increasing monomer solubility leads to A-B copolymers with random-blocky co-monomer sequences.

C1.00070 Computer simulation of formation of random-blocky diblock copolymers in dilute solutions . JESSE BOER, APICHART LINHANANTA, Department of Physics, Lakehead University — The formation of micelles and vesicles in dilute solutions of amphiphilic diblock copolymers is investigated by the real-space self-consistent field theory (SCFT) in two dimensions and by a Monte Carlo lattice model in three dimensions. The real-space SCFT method produced rodlike and spherelike micelles and vesicles. It is found that the shapes of the microstructures are determined by the initial conditions in the SCFT algorithms, and that, in general, vesicles have lower free energy than micelles. In contrast, the Monte Carlo simulation of the lattice model, it is found that as the volume fraction of copolymer increases, the microstructure go from spherelike micelles to rodlike micelles to vesicles and, at high fraction, to the lamellar phase.

1We acknowledge the financial support of the National Sciences and Engineering Research Council of Canada.
Secondary Forces as a Driving Mechanism for Thermally Induced Drug Release in ROMP based Polymers, CASEY KIMBALL, SHAW L. HSU, GREG TEW. University of Massachusetts Amherst — To control drug release via a thermal mechanism is important from both a fundamental and application standpoint. Traditionally, biocompatible polymers with secondary interactions in the backbone have been investigated. Instead, we have synthesized a novel poly(ethylene oxide) crosslinked Ring Opening Metathesis Polymerization based polymer comprised of a polyboroborone derived backbone with multiple substituent groups, including a tetra-ol, diamine, dicarboxylic acid and amino acid based side chains. The strength of secondary interactions based on the functional groups present plays a critical role in chain dynamics and thermal properties. DSC measurements revealed a substantial change in the thermal transitions to be as high as thirty degrees, depending on substituent group and crosslinking properties. Inspired spectroscopy has been employed to characterize the functional groups present. It has been revealed that the strength of the hydrogen bonds is strongly correlated with the transition temperature. Additionally, the presence of water has a perturbing effect of disrupting the hydrogen bonding network and affecting the chain dynamics of the overall crosslinked system.

DNA Electrophoresis using entropic trapping, HAOBIN LUO, DILIP GERSAPPE, Dept of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794 — We examine the effects of surface patterning on DNA electrophoresis. Using chemically patterned stripes of different widths we can control the separation of DNA. Due to entropic trapping of the chains on the stripes, depending on the width of the stripe and the length of the DNA, we show (using MD simulations) that it is possible to separate chains in increasing order of length and in decreasing order.

We show an experimental realization of this effect and illustrate how DNA motion on the surface can be influenced by both the width of the stripe and the periodicity of the pattern.

Protein adsorption at calcium oxalate monohydrate crystal surfaces, J. WESSON, Department of Veterans Affairs, X. SHENG, Abbott Laboratories, J. RIMER, New York University, T. JUNG, Seoul University, M. WARD, New York University — Calcium oxalate monohydrate (COM) crystals are the dominant inorganic phase in most kidney stones, and kidney stones form as aggregates of COM crystals and organic material, principally proteins, but little is known about the molecular level events at COM surfaces that regulate COM aggregation. We have examined the influence of polyelectrolytes on the force of adhesion between chemically modified atomic force microscopy (AFM) tips and selected COM crystal faces in saturated solution. In general, we found that polyanions bind to COM surfaces and block adhesion of a carboxyfunctionalized AFM tip, while polycations had no measurable effect on adhesion force under the same conditions. We did observe a unique absence of interaction between poly(glutamic acid) and the COM (100) face compared to other synthetic polycations, and some native urinary protein structures also exhibited unique face selective interactions, suggesting that simple electrostatic models will not completely explain the data.

Phase Transitions in Superparamagnetic Polymer Brush Particles, ANNETTE SCHMIDT, Heinrich Heine-Universitaet Duesseldorf, ANDREAS KAISER, Heinrich Heine-Universitaet Duesseldorf — Nanostructured inorganic / organic hybrid materials play an outstanding role in modern technology. We present results on the synthesis and characterization of novel thermo- and magnetoresponsive polymer brush coated particles. The investigated system is composed of nanocrystalline magnetite (Fe3O4) as an inorganic core and a covalently anchored polystyrene (PS) shell. In cyclohexane, a thermostressive magnetic fluid is obtained due to a critical solution behaviour of the PS arms. Cyclohexane. Beside the phase transition of Fe3O4@PS particles, the well known coil-to-globule transition of Fe3O4@PS particles in cyclohexane is investigated. Both phenomena are compared to the behaviour of linear polymeric brushes. The presented results show that magnetic brush particles are well-suited as a model system for the investigation of temperature transitions of surface-attached polymers.

3D Analysis of Lattice Defects in the Gyroid Network Structure of a Block Copolymer/Homopolymer Blend, SATOSHI AKASAKA, TETSURO OKAMOTO, VINCENT H. MAREAU, HIROKAzu HASEGAWA, Department of Polymer Chemistry, Kyoto University — The bicontinuous microdomain structures known as gyroid cubic phase (a = 3d) can be observed in a narrow composition region of a block copolymer system. In the study of the casting process of the polystyrene-block polysoprene (SI)/homopolystyrene (hS) blend with a particular composition from toluene solution, we observed that sponge phase, an irregular network structure, transformed into gyroid phase by expelling excess hS outside of the gyroid grains. During the growth of the gyroid grains, a variety of interesting lattice defects appear due to the remaining excess hS in the grains. Such defects may be useful in designing photonic band-gap devices based on gyroid cubic phase if we can control them. However, the analysis of the defect structures in gyroid network is not easy since gyroid network itself is too complex. So, we employed a novel technique, electron tomography, to visualize the 3D defect structures in gyroid network. In this presentation, we demonstrate how useful it is and clarify the defects structure in 3D

Phase Behavior of Polymer Blends Containing End-Associating Polymers, MICHELLE WRUE, MITCHELL ANTHAMATTEN, University of Rochester — Polymer blending is an important route to the creation of new polymeric materials with superior processing and tunability. We are studying the effects of strong, site-specific, hydrogen-bonding groups on the phase behavior of traditional polymer blends exhibiting upper critical solution temperature (UCST) behavior. Ureidopyrimidinone (UPy) functional groups self-associate through the formation of four hydrogen bonds. We have synthesized telechelic telepolyureidopyrimidinone (TPU-P and TPY-P) and poly(4-methyl styrene) (P4MS). We have characterized these materials in ternary polymer-polymer-solvent systems to investigate the miscibility of blends containing UPy-functionalized polymers. Polymer pairs studied include PS/polybutadiene (PS) and PB/P4MS. Phase behavior and end-association were studied using laser light scattering and dilute solution viscometry. Data from PS/PB/toluene blends containing only one functionalized polymer, PS, indicate a reduction in miscibility relative to the corresponding parent blend. PS/P4MS blends in which both polymer components contain the UPy functional group are also being studied.

Self-assembly of rod-coil block copolymers from weakly to moderately segregated regimes, RAFFAELE MEZZENGA, NICHOLAS SARY, University of Fribourg, Physics Department, GEORGES HADZIOANNOU, CYRIL BROCHON, University Louis Pasteur, France — We report on the self-assembly behaviour of two homologue series of rod-coil block copolymers in which, the rod, a π-conjugated polymer, is maintained fixed in size and chemical structure, while the coil is allowed to vary both in molecular weight and chemical nature. This allows maintaining constant the liquid crystalline interactions, expressed by Maier-Saupe interactions, ω, while varying the tendency towards microphase separation, expressed by the product between the Flory-Huggins parameter and the total polymerization degree, ΧN. Therefore, the systems presented here allow testing directly some of the theoretical predictions for the self-assembly of rod-coil block copolymers in weakly segregated regime. The two rod-coil block copolymer systems investigated, were poly(DEP-phenylenevinylene-b-styrene), whose self-assembly takes place in the very weakly segregated regime, and (DEP-phenylenevinylene-b-4vinylpyridine), for which self-assembly behaviour happens under increased tendency towards microphase separation, hereby referred as moderately segregated regime. Experimental results for both systems are compared with predictions based on Landau expansion theories.

Self-Organization on Multiple Length Scales in “Hairy-Rod”–Coil Block Copolymer Supramolecular Complexes, RAFFAELE MEZZENGA, MATTHEW HAMMOND, University of Fribourg, Physics Department, HARM-ANTON KLOK, EPFL, Lausanne — A peptide-synthetic hybrid block copolymer, poly(ethylene oxide)-block-poly(L-glutamic acid), is demonstrated to form supramolecular complexes with primary alkylamines of varying alkyl chain length (8 to 18 methylene units) in organic solvents via acid-base proton transfer and subsequent ionic bonding. The peptidic block being in the α-helical conformation, these materials behave as coil–“hairy rod” block copolymers, and show hierarchically self-organized nanostructures in the solid state; X-ray scattering measurements show mesomorphic behavior at the length scales of both the overall block copolymer and the polypeptide-alkylammonium complex.
C1.00079 Self-Consistent Field Theory Simulations of Confined 2D Block Copolymer Thin Films, SU-MI HUR, GLENN FREDRICKSON, UC Santa Barbara, AUGUST BOSS, EDWARD KRAMER, CARLOS GARCIA-CERVERA, UC Santa Barbara — We present self-consistent field theory (SCFT) simulations of block copolymers confined in a square well in order to guide self-assembly towards defect-free in-plane arrays. In particular, tetragonal (square) packing, which is thought to be crucial to developing novel information storage and electronic devices, has been observed in simulations of thin films of AB diblock copolymers with suitable A homopolymer additives confined in square wells. While the A-B + A system only supports square lattices of limited sizes (up to 4x4), we were able to produce large-area defect-free square lattices using blends of chemically different diblock copolymers with suitable attractive interactions between blocks. Our simulations demonstrate that order originates at the walls and then permeates throughout the system.

C1.00080 Orientation Control of Diblock Copolymer Thin Films by the Addition of Amphiphilic Surfactants, JEONG GON SON, KOOKHEON CHAR, Seoul National University, PAUL F. NEALEY, HUIMAN KANG, University of Wisconsin — The precise control of the orientation of block copolymer (BCP) thin film is crucial to fully exploit the potential of these materials for applications in nanotechnology. The orientation control is, however, challenging as BCP nanodomains spontaneously self-assemble in a configuration that minimizes the total free energy of the system. The perpendicular orientation of BCP domains, in particular, has potential for device applications. In this presentation, we would like to introduce a new approach for the perpendicular orientation of BCP domains from the top of a BCP film toward a bottom substrate. Our concept is based on the properties of surfactants that naturally locate at interfaces to tailor the surface properties of materials. We demonstrate how the segregation of low molecular weight surfactants, oleic acid (OA) in present case, at the top surface of a PS-b-PMMA BCP thin film can easily create energetically neutral conditions for the BCP, resulting in the desired perpendicular orientation. The main advantage of this new approach is that nano-scale patterns can be generated at the top of a BCP film after short annealing time on any substrates. We verified the structures and mechanisms of the surfactant-assisted perpendicular orientation of thin block films using AFM, SEM, GISAXS and Neutron Reflectivity.

C1.00081 Diblock copolymer thin films: Compressed fluid induced order, PETER GREEN, ABRHAM ARCEO, University of Michigan — We show that liquid and super critical CO2 induces long-range order into thin film, symmetric, polystyrene-b-polymethylmethacrylate (PS-b-PMMA) diblock copolymers, supported by SiO2/Si substrates, in a temperature range where both bulk and thin films of these materials remain ordered. Under vacuum conditions the substrate induces order the thin films at temperatures significantly above the bulk order-disorder transition temperature. Ordering occurs at $N \approx 7.94$, where $N$ is the Flory-Huggins interaction parameter and $N$ is the degree of polymerization, which is below the bulk value of $N_{bulk} = 10.5$. In the presence of CO2, the transition shifts to yet lower values of $N$, indicating a more significant degree of incompatibility between the PS and PMMA systems of $N > 10.5$ become phase mixed in the presence of liquid or super critical CO2.

C1.00082 Crystal Orientation of Polyethylene oxide in a Defect-Free 1D Confined System of Polyethylene oxide-b-Polystyrene Diblock Copolymer Single Crystals, MING-SIAO HSIAO, JOSEPH X. ZHENG, RYAN M. VAN HORN, RODERICK P. QUIRK, STEPHEN Z. D. CHENG, The University of Akron, BERNARD LOTZ, EDWIN L. THOMAS, HSIN-LUNG CHEN, THE UNIVERSITY OF AKRON TEAM, MIT COLLABORATION, INSTITUT CHARLES SADRON COLLABORATION, NATIONAL TSING-HUA UNIVERSITY COLLABORATION — Highly oriented crystalline-amorphous block copolymers under a large amplitude shear open a window for studying crystal orientation evolution within a one-dimensional confined environment at different degrees of supercooling, however, inevitable defects and internal stresses are the main cause of releasing the confinement effect on crystal polymeric orientation, which is a 1-D confined lamellae of 10 nm PS-b-PBEO solution grown single crystal were used to study the crystal orientation evolution as a function of crystallization temperature (Tcr) via recrystallization. From DSC and temperature dependent SAXS, it was found that a high quality PS layers can induce the formation of oriented crystals, which is in good agreement with the recent model of some groups. In this paper, we report a detailed analysis of this and other systems, which can be described as the model of a charge transport in confined polymer systems, which are used as a foundation for other research.

C1.00083 Well-Defined Fullerene-Containing Diblock Copolymers Based on Regioregular Poly(3-hexylthiophene) and Poly(methyl methacrylate): Synthesis and Photovoltaic Properties, JEA UK LEE, WON HO JO, Materials Science and Engineering, Seoul National University, ALI CIRPAN, TODD EMRICK, THOMAS RUSSELL, POLYMER SCIENCE AND ENGINEERING, UNIVERSITY OF MASSACHUSETTS — Polymeric solar cells based on conjugated polymer and fullerene materials have opened a new avenue to develop economically renewable energy resources. Recently, bulk heterojunction solar cells fabricated by simplifying blending regioregular poly(3-hexylthiophene) with fullerene derivatives have resulted in great improvement in the power conversion efficiency. Although a remarkable progress has been made, bulk heterojunction solar cells still have several problems. First, in all of the bulk heterojunction solar cells, the conjugated polymer and electron acceptor have been randomly intermixed throughout the film. Second, the blend of conjugated polymer and fullerene derivatives usually results in a morphophase separation, limiting the charge separation and thus the power conversion efficiency in a photovoltaic device. We have designed and synthesized novel diblock copolymers composed of regioregular poly(3-hexylthiophene) and fullerene containing poly(methyl methacrylate) (PMMA). The diblock copolymers self-assemble into nanostructured morphologies (lamellae or hexagonally packed cylinder), which provide exons with large interfaces for charge separation on the nanometer scale.

C1.00084 Point Mutations Effects on Charge Transport Properties of the Tumor-Suppressor Gene p53, RUDOLF A. ROEMER, Department of Physics and Centre for Scientific Computing, University of Warwick, UK, CHI-TIN SHIH, Department of Physics, Tunghai University, Taiwan, STEPHAN ROCHE, CEA/DSM/DRFMC/SPSMS Grenoble, France — We report on a theoretical study of point mutations effects on charge transport properties in the DNA sequence of the tumor-suppressor p53 gene. On the basis of effective tight-binding models which simulate hole propagation along the DNA, a statistical analysis of mutation-induced charge transfer modifications is performed. In contrast to non-cancerous mutations, mutation hotspots tend to result in significantly weaker changes of transmission properties. This suggests that charge transport could play a significant role for DNA-repairing deficiency yielding carcinogenesis.

1 CTS (National Science Council grant 95-2112-M-029-003), RAR (Leverhulme grant F/00215/AH)

C1.00085 Endohedral Fullerenes in Organic Thin Film Photovoltaic Devices, RUSSEL ROSS, EDWARD VANKEUREN, Georgetown University, MARTIN DREES, CLAUDIA CARDONA, BRIAN HOLLOWAY, Luna Nanoworks, DIRK GULDI, Friedrich-Alexander-Universitat Erlangen-Nurnberg — Cost factors in inorganic solar cells have opened up a new path to less expensive manufacturing techniques using bulk heterojunction polymer/fullerene based solar cells. Using empty cage fullerene derivatives as the acceptor material, state-of-the-art organic photovoltaics currently display ~5% overall conversion efficiency. One of the main factors limiting the efficiency in organic solar cells is the low open circuit voltage. The open circuit voltage is governed by the molecular orbitals of the donor and acceptor material; therefore better matching of the orbitals will lead to improved voltages. We present a novel acceptor material based on TRIMETASPHHERE® carbon nanomaterials (TMS). TMS are endohedral metallofullerenes that consist of a trivalent nitride cluster enclosed in a C80 cage. First-generation TMS derivatives have been synthesized; electrochemical and photophysical studies show behavior consistent with C60 but with improved molecular orbitals. The electrochemical data suggests a maximum voltage increase of up to 280 mV over C60-PCBM-based devices. Organic solar cell devices are currently under construction and performance results will also be presented.

3 AFRL MANTECH program (contract # USAF571004C0001) & AFOSR (contract # FA9550-07-C-0050).
C1.00086 Multilayer polymer light emitting diode (PLED) devices studied using resonant soft x-ray reflectivity. CHENG WANG, B. WATTS, T. ARAKI, H. ADE, NCSU, A. HIXEMER, LBNL, A. GARCIA, T.-Q. NGUYEN, G.C. BAZAN, K.E. SOHN, E.J. KRAMER, UCSB — The performance of multilayer PLED devices is likely to be strongly affected by the structure of the interface between the active layers. Using resonant soft x-ray reflectivity (RSoXR), the contrast between polymer components can be greatly enhanced by tuning the photon energy to absorption resonances near 285 eV and the interfacial width can be measured. The interfacial widths of model bilayers of poly(9,9-bis(6’-N,N,N-trimethylammoniumhexyl)fluorene-co-alt-1,4-phenylene bromide) (PFNBr)/poly(2-methoxy-5-(2’-ethylhexyloxy)-p-phenylene vinylene) (MEH-PPV) on SiO2 substrates were manipulated by changing the sample preparation process and were measured by RSoXR, allowing w to be correlated to device performance. In addition, for a real PLED device with a more complicated multilayer structure, but missing the top Al electrode, it was demonstrated that the top four interfaces can be fully characterized using RSoXR, adjusting the material contrast in order to selectively observe different layers by tuning to different photon energies.

C1.00087 Breath Figure Templated Assembly of Ordered and Disordered Array of Holes in Polymer Films. VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, SAI M. GOGNENI, MATIJA CRNE, School of Chemistry and Biochemistry, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332 — Breath figures are patterns formed when water vapor from our breath condenses over a cold substrate. These patterns, which mimic the behavior of dew or chemical vapor deposition, comprise of drops with range of self-similar sizes, and form through coalescence assisted growth. Water drops that condense over evaporating polymer solutions can organize into close packed arrays, and template nicely ordered arrays of holes in polymer films. Using experiments and theory, we examine the role of various parameters that contribute to the formation of ordered assembly. We will present our findings about how the choice of polymer and polymer concentrations and air flow conditions influences the extent of order and the pore size.

C1.00088 Carbon nanotube based gecko inspired self-cleaning adhesives. SUNNY SETHI, LIEHUI GE, The University of Akron, PULICKEL AJAYAN, Rensselaer Polytechnic Institute, DHINOWALA ALI, The University of Akron — Wall climbing organisms like geckos have unique ability to attach to different surfaces without use of any viscoelastic material. The hairy structure found in gecko feet allows them to obtain intimate contact over a large area thus allowing them to adhere using van der Waals interactions. Not only high adhesion, the geometry of the hairs makes gecko feet self-cleaning, thus allowing them to walk continuously without worrying about loosing adhesive strength. Such properties if mimicked synthetically could form basis of a new class of materials, which, unlike conventional adhesives would show two contradictory properties, self-cleaning and high adhesion. Such materials would form essential component of applications like wall climbing robot. We tried to synthesize such material using micropatterned vertically aligned carbon nanotubes. When dealing with large areas, probability of defects in the structure increase, forming patterns instead of using uniform film of carbon nanotubes helps to inhibit crack propagation, thus gives much higher adhesive strength than a uniform film. When carbon nanotube patterns with optimized aspect ratio are used, both high adhesion and self cleaning properties are observed.

C1.00089 Understanding the Structure and Phase Behavior of Model DNA-Linked Nanoparticles by Monte Carlo Simulations. JUAN ARAQUE, Rice University, ATHANASSIOS PANAGIOTOPoulos, Princeton University, MARC ROBERT, Rice University — The high specificity and selectivity of DNA hybridization makes nucleic acid recognition a powerful tool for bottom-up assembling approaches. Here, we propose a coarse-grained model to address the question of how nanoparticles tethered with single stranded DNA self-assemble in solution. Our approach employs a computationally efficient discretization of hard-core interactions and a high-coordination lattice, in combination with parallel tempering and multicanonical Monte Carlo simulations. This simplified model of DNA strands not only accounts for all physically relevant interactions, but also enables an significant reduction of the problem dimensionality. We discuss the effects of a number of system parameters and assembling architectures on the equilibrium structures and phase behavior. In addition, we establish the relation of these results with experimental observations.

C1.00090 Relationship Between Interfacial Strength and Materials Properties in Hybrid Organic/Inorganic Nanomaterials. CHAD SNYDER, MICKEY RICHARDSON, JING ZHOU, GALE HOLMES, ALAMGIR KARIM, NIST Polymers Division, NANDIKA D’SOUZA, University of North Texas, Dept. of Materials Science and Engineering — Thermal interface materials (TIM’s) are critical to the semiconductor electronics industry for heat dissipation, a potential show-stopper for future technology nodes. Essentially, an epoxy nanocomposite, TIMs suffer from a series of typical nanocomposite limitations including heat conduction in nanoscale inclusions, nanoparticle dispersion, void formation with thermal cycling, and interfacial resistance between the matrix and filler. It is postulated that the interfacial adhesion between the matrix and nanofiller is at the root cause of many of these difficulties, however, few techniques exist to characterize this critical property. Compounding this are the overall difficulties associated with characterizing these materials in their ultimate applications, i.e., thin films. To this end, a novel series of organic/inorganic hybrid nanostructured materials based on layered double hydroxides in epoxy matrices were designed as a test bed to develop the measurement techniques needed to elucidate the relationship between the material structure and dynamics and the ultimate materials properties. Initial results are presented based on characterization by mechanical, dielectric, and thermal spectroscopies.

C1.00091 Control of Polymer Translocation with External Forcing. SANTTU OLLILA, Helsinki University of Technology, Finland, KAIFU LIO, TAPIO ALA-NISSILA, Helsinki University of Technology, SEE-CHEN YING, Brown University — We investigate the dynamics of driven polymer translocation through a nanopore using two-dimensional Langevin dynamics simulations within the bead-spring model. A pulling force F is exerted on the first monomer whilst there is an opposing force F_{E_0} in the pore. For this setup, we calculate the distribution of translocation time τ, which is defined as the time for the polymer to traverse from one side of the membrane to the other, and the waiting time t_{W}, which is defined as the time between the translocations of the i-th and the (i+1)-th bead. As our main result, we characterize the fluctuations and the positions of the beads along the direction of F with respect to the position of the segments in the nanopore, and with respect to the position of the pore. Implications of these results to actual sequencing experiments are discussed.

C1.00092 Structural Relaxation of Stacked Ultrathin Polystyrene Films. YUNG P. KOH, SINDEE L. SIMON, Texas Tech University — The kinetic behavior of stacked polystyrene ultrathin films is investigated by differential scanning calorimetry (DSC) and compared to the behavior of bulk polystyrene. The fictive temperature (T_f) was measured as a function of cooling rate and as a function of aging time for aging temperatures below the nominal glass transition temperature (T_g). The stacked thin films show enthalpy overshoots in DSC heating scans which are reduced in height but occur over a broader temperature range relative to the bulk response for a given change in fictive temperature. The cooling rate dependence of the limiting fictive temperature, T_f', is also found to be higher for the stacked thin film samples; the result is that the magnitude of the T_g depression between the thin film samples and the bulk is inversely proportional to the cooling rate consistent with other results in the literature. We also find that the rate of physical aging of the stacked thin films is comparable to the bulk when aging is performed at the same distance from T_g; however, when conducted at the same aging temperature, the thin film samples show accelerated physical aging due to their depressed T_g values. This result is in contrast to recent work in the literature on PMMA ultrathin films and on o-TP confined in nanopores.
Surface Dynamics Of Homopolymer Brushes

C1.00093

MARK D. FOSTER, The University of Akron, Akron, OH 44325-3909 — The surface dynamics of polystyrene (PS) and poly(n-butyl acrylate) (PnBA) homopolymer brushes were investigated by X-ray photon correlation spectroscopy for the first time. Within the range of time (0.2 - 1100 s) and length scale (0.2-5 nm) studied, no fluctuations of the brush surfaces were detectable. When PS brushes of thicknesses in the range of 9-101 nm and high grafting density (>0.5 chains/nm²) were considered at temperatures up to Tg+130°C, no relaxation was visible within our window of in-plane wave-vector. Even reduction of the grafting density from 0.6 to 0.1 chains/nm² did not bring the relaxation into the window. Likewise, no relaxation was observed for PnBA brushes up to 170°C above Tg. The suppression of surface fluctuations is a result of covalent tethering.

Mass Transport through Dynamic Polymer Networks Containing Reversibly Associating Side-Groups

C1.00094

JIAHUI LI, ANDREW HILMER, MITCHELL ANTHAMATTEN, Department of Chemical Engineering, University of Rochester, HUNG CHUNG, JAMES MCGRATH, Department of Biochemical Engineering, University of Rochester — Dynamic polymer networks containing both covalent crosslinks and reversibly associating side-groups were synthesized. Those polymers exhibit novel shape-memory properties due to strong temperature dependence of side-group association. Diffusion of different molecules through polymer networks were studied using three techniques: gravimetric sorption, dye permeation, and fluorescence recovery after photo-bleaching. The dependence of diffusion on temperature, network architecture, solute size, and the interaction between the solute and the network will be discussed. Results show polymer networks with reversibly associating side-groups exhibit unusually strong temperature dependence. This study highlights the potential of these and other dynamic networks to serve as precision drug or reagent release devices.

Nanoscale building blocks for the development of novel proton-exchange membranes

C1.00095

XIAORONG WANG, Bridgestone Americas, Center for Research and Technology, 1200 Firestone Parkway, Akron, OH 44317-0001, USA. Email: WangXiaorong@BFUSA.com — The reinforcement of nano-sized polymeric hard core-hairy shell particles in a polymer matrix of chemically identical chains was investigated by dynamical mechanical measurements. We found that the magnitude of reinforcement depended strongly on the phase behavior of the nanoparticles in the polymer matrix. In one phase region, the mechanical response was nearly linear, and the reinforcement was approximately described by the Guth-Smallwood relationship in terms of filler concentration. In two phase region, however, the mechanical response was largely nonlinear, even for strain lower than 1%, and the reinforcement at low strains was an exponential function of the filler concentration. We show that by tailoring the filler interaction potentials the entire reinforcing mechanism can be changed.

Meso-scale modeling of block copolymer/colloid nano-composites

C1.00096

MARCO PINNA, School of Computing, Engineering and Physical Sciences, University of Central Lancashire, Preston, UK, IGNACIO PAGONABARRAGA, Department of Fundamental Physics, University of Barcelona, Spain, ANDREI ZVELINDOVSKY, Centre for Materials Science, University of Central Lancashire, Preston, UK — We develop a coarse grained simulation technique to study dynamics in soft nano-composites. The system consists of block copolymer melt or solution with nano-size colloidal particles. The time evolution of the system is described by a multiscale approach: a field based simulation for block copolymer component and a particle based method for nano-cohoids. The block copolymer is modelled by cell dynamics simulation technique, and colloids are modelled in a spirit of dissipative particles dynamics. A cross interaction term is controlling the interplay of dynamics of both components. The influence of colloids on block copolymer morphology is investigated.

Fundamentals of the reinforcement of hairy nanoparticles in rubber compunds

C1.00097

XIAORONG WANG, Bridgestone Americas, Center for Research and Technology, 1200 Firestone Parkway, Akron, OH 44317-0001, USA. Email: WangXiaorong@BFUSA.com — The reinforcement of nano-sized polymeric hard core-hairy shell particles in a polymer matrix of chemically identical chains was investigated by dynamical mechanical measurements. We found that the magnitude of reinforcement depended strongly on the phase behavior of the nanoparticles in the polymer matrix. In one phase region, the mechanical response was nearly linear, and the reinforcement was approximately described by the Guth-Smallwood relationship in terms of filler concentration. In two phase region, however, the mechanical response was largely nonlinear, even for strain lower than 1%, and the reinforcement at low strains was an exponential function of the filler concentration. We show that by tailoring the filler interaction potentials the entire reinforcing mechanism can be changed.

Thermoporosimetric Measurements of Network Heterogeneity: Melting Point Depression

C1.00098

JINRONG WU, GREGORY MCKENNA1, Department of Chemical Engineering, Texas Tech University — To improve understanding the heterogeneity and structure of polymer networks, thermoporosimetry was performed on four model networks of polydimethylsiloxanes (PDMS), which were obtained by tetrakis(dimethylsiloxy)silane crosslinking vinyl terminated PDMS having different molecular weights. The effects of solvent molecular size, solvent quality and PDMS chain length between cross-links on the anomalous melting point depression of solvents in these model networks were systematically investigated. The results are analyzed in terms of both the Gibbs-Thomson (GT) equation and the Flory-Huggins (FH) model. Furthermore, we also compared the the pore size distributions obtained from thermoporosimetry for these model networks with the molecular distribution of their oligomers as determined by Matrix Assisted Laser Desorption/Ionization Time of Flight Mass Spectrometry.

1 Corresponding author

Statistics and dynamics of blends of linear and ring polymers

C1.00099

MICHAEL LANG, Leibniz-Institute for Polymer Research, MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina, 27599 Chapel Hill, N.C., USA — This work focuses on conformations and dynamics of blends of linear and ring polymers. Rings in a melt of homo-polymer rings are compressed due to topology, if rings are significantly larger than the entanglement length. Dilute rings with degree of polymerization, N_1, immersed in a melt of linear polymers with degree of polymerization, N_2, are almost ideal if N_1 > N_2^{1/2} and swell if N_1 < N_2^{1/2}. Dynamics of pure ring melts is enhanced as compared to pure linear melts. Thus, minority of linear chains immersed in ring melt experiences enhancement of diffusion and relaxation. On the other hand, minority of long entangled rings immersed in melt of long entangled linear chains gets temporarily trapped. This leads to a clear reduction in diffusion coefficient while keeping relaxation (as determined by half ring relaxation) almost unaffected.
C1.00100 Spectroscopic Analysis of Amorphous Structure in Fluorinated Polymers, SHAW L. HSU, YUNING YANG, SURIYAKALA RAMALINGAM, University of Massachusetts Amherst — High-quality polarized Raman spectra have been obtained for various poly(vinylidene fluoride) (PVDF) structures, crystalline and amorphous. These data encouraged us to revisit the Raman band assignment, especially within the conformational sensitive region (400-1100 cm\(^{-1}\)) and use the new understanding to characterize the amorphous region. Vibrational bands have been assigned on the basis of observed polarization characteristics and the calculated potential energy distribution (PED). The simulated results agree well with the experimental polarized Raman study. On the basis of the calculated PED, combined with simulation of different conformational sequences (tttt, ttggt, tggg, gggg), spectroscopic features (band intensity at 648 cm\(^{-1}\) and the frequency change of the 856 cm\(^{-1}\) band) were associated with the distribution of rotational isomeric states. Two rotational isomeric state (RIS) models were analyzed and compared in the simulation study of the amorphous state. On the basis of the spectroscopic features of experimental and simulated Raman spectra, the conclusion was reached that the model which predicts a higher gauche population more accurately describes the amorphous state. This analysis provides an opportunity to describe the amorphous state in a quantitative manner.

C1.00101 Equilibrium Pathway of Spin-coated Polymer Films, OPHELIA TSUI, Physics Department, Boston University, Boston, MA02215, YONG JIAN WANG, Physics Department, Hong Kong University of Science & Technology, Clear Water Bay, Hong Kong, FUK KAY LEE, Physics Department, Boston University, Boston, MA02215, C.-H. LAM, Department of Applied Physics, Hong Kong Polytechnic University, Hung Hom, Hong Kong, ZHAOHUI YANG, Physics Department, Boston University, Boston, MA02215 — Spin-coating is a common method of making thin polymer films. Recent experiments show that polymer films produced by this method are highly non-equilibrated. By monitoring the temporal evolution of the surface structure of freshly sin-cast polystyrene films on Si with molecular weights, 2.3 ≤ M\(_{\text{w}}\) ≤ 393 kg/mol, we find that the relaxations can be fully accounted for by thermal excitations of surface capillary waves on the film surface. Modeling of the data based on this relaxation scheme leads to excellent agreement between the viscosity of the films and that of the bulk polymers. Our results provide compelling evidence that thickness uniformity is the major cause of the non-equilibration of the films.

1 We are grateful to the support of NSF through the project DMR-0706906.

C1.00102 COMPLEX STRUCTURED MATERIALS —

C1.00103 Crystal structures and physical properties of nanostructured [(PbSe)\(_{0.99}\)\(_{m}\)(WSe\(_2\))\(_n\)] (m, n=1-5), QIYIN LIN, Materials Science Institute, University of Oregon, Eugene, Oregon 97403, COLBY HEIDEMAN, CLAY MORTENSEN, NGOC NGUYEN, DAVID C. JOHNSON, Materials Science Institute, University of Oregon, Eugene, Oregon 97403, PAUL ZSCHACK, Advanced Photon Source, Argonne National Laboratory, Argo, IL 60439, CATALIN CHIRITEASCU, DAVID G. CAHILL, Department of Materials Science and Engineering, University of Illinois, Urbana, IL 61801. — We report a class of nanostructured mist layer compounds [(PbSe)\(_{0.99}\)\(_{m}\)(WSe\(_2\))\(_n\)] (m,n=1-5) synthesized using a modulated elemental reactant technique. The structures are built of two subsystems alternately stacking along the c direction - a distorted rock salt structure (PbSe)\(_5\) and a transition metal dichalcogenide (WSe\(_2\)). These nanostructured compounds have ultra low thermal conductivities, as small as 0.06 Wm\(^{-1}\)K\(^{-1}\), which can be attributed to the structural mist between the components resulting in an unusual balance of order and disorder. Annealing samples under different partial pressures of selenium can be used to control electrical conductivity and the value of the Seebeck coefficient. The relationship between nanostructures and physical properties will be discussed.

The corresponding author

C1.00104 Low Temperature Study of Mechanically Alloyed EuFeO\(_3\), SUMAN KATHIWADA, DEREJE SEIFU, Morgan State University — Rare-earth (R) and transition metal (T) perovskite Oxides RTO\(_3\) are of great interest in Physics, besides potential applications in variety of devices. Here, we present study of EuFeO\(_3\) synthesized by mechanical alloying. The Mössbauer measurement on EuFeO\(_3\) is one of the rare cases where both the R and the T sites are probed in the same compound. Room temperature Mössbauer study is already reported [1], here we report low temperature Mössbauer measurements. Measurements indicate that hyperfine magnetic field increased with decreasing temperature. The \(^{157}\)Fe Mössbauer spectra depicts that there is only a magnetic sextet at 20K implying pure ferromagnetic state. As temperature increased two non-magnetic states appeared and their propensity increased with temperature. The \(^{157}\)Eu Mössbauer measurements show that the line width at half maxima has a peak between 50K and 100K. [1] Seifu, D., Takacs, L., Kebede, A., “Mössbauer Study of Mechanically Alloyed EuFeO\(_3\).” J. of Mag. and Mag. Matt., 302, pp 479 – 483, 2006.

1 Supported by ARL, WMRD, Aberdeen Proving Ground W1813LT-5006-7056.

C1.00105 Production of metal cluster patterns using Focused Ion Beams (FIB), FARHAD GALEH, NIKLAS GRÖNHAGEN, HEINZ HÖVEL, Technische Universität Dortmund, Experimentelle Physik I, Germany, LARS BRUCHHAUS, SVEN BAUERDICK, JÜRGEN THIEL, RALF JEDE, Raith GmbH, Dortmund, Germany — Nanometer sized pits on graphite (HOPG) substrates can be used as nucleation centers to produce clusters with a narrow size distribution. In previous experiments [1] nanometer sized pits were produced by sputtering and oxidizing the sample. As a result we get nanoparticles which are a few nanometers wide and only one monolayer deep, distributed at random locations on the surface. In the present study a focused beam of gallium ions is used to produce nanoparticles in a given pattern on the substrate. The FIB instrument (Raith ionLine) is capable of a resolution below 10 nm [2]. Using the nanoparticles as nucleation centers we are able to produce gold islands as well as silver clusters in a given pattern by depositing metal atoms. Furthermore the nanopatterning on the surface in combination with Monte Carlo simulations helps investigating the ion beams, e.g. ion distribution, recoils as well as the penetration depth of the ions [3]. In this respect the oxidation of HOPG-samples provides a method to study the ion impact effects. [1] H. Hövel, Appl. Phys. A 72 (2001) 295; [2] J. Gierak et al., Appl. Phys. A 80 (2005) 187; [3] F. Gahle, R. Köster, H. Hövel, L. Bruchhaus, S. Bauer, J. Thiel, R. Jede, J. Appl. Phys. 101 (2007) 044301.

C1.00106 The role of low frequency vibrational modes localization properties in the glass transition and mechanical stability of glasses, GERARDO NAUMIS, Depto. de Física-Química, Instituto de Física, UNAM — It is surprising that although glasses present low frequency vibrational anomalies like floppy modes or the Boson peak, not so much effort has been made in order to understand the relationship between glass transition and low frequency anomalies, which we know are fundamental in the stability of solids. We will show that rigidity theory allows to understand in a systematic way such relationship. Then, the effects of flexibility and chemical composition in the variation of the glass transition temperature are obtained by using the Lindemann criteria, that relates melting temperature with atomic vibrations, and rigidity theory. Using this criteria and that floppy modes at low frequencies enhance in a considerable way the average quadratic displacement, we show that the consequence is a modified glass transition temperature. This approach allows to obtain in a simple way the empirically modified Gibbs-DiMarzio law, which has been widely used in chalcogenide glasses to fit the changes in the glass transition temperature with the chemical composition [1]. The method predicts that the constant that appears in the law depends upon the ratio of two characteristic frequencies (or temperatures). This constant is estimated for the Se\(_{1-x}\)As\(_{1-x}\)\(_{2-y}\)\(_{y}\) glass by using the experimental data of vibrational states, and the result shows a good agreement with the experimental fit from glass transition temperature variation. [1] G.G. Naumis, Phys. Rev. B 73, 172202 (2006).
Glassy systems under confinement have been studied with great enthusiasm and effort for the last decades. They are relevant both fundamentally and technically because there is still debate about the nature of glass transition in small geometries which is important for lithographic processes in the semiconductor and other industries. In this work we are using the Wang-Landau approach also known as Density of States Monte Carlo to study glassy systems in bulk and under confinement. We apply the technique to a model binary Lennard Jones glass as well as the small organic glass former Ortho-terphenyl (OTP). For Lennard Jones glasses we use a well tested model. For OTP we start from a united atom model and then derive systematically a coarse grained representation by replacing each phenyl ring with a bead and using the Iterative Boltzmann Inversion. The properties of bulk Lennard Jones model show very good agreement with literature values. The atomistic and coarse grained representations of ortho-terphenyl in the bulk are in good agreement with experiments. Unsupported freestanding films show a lower glass transition than the bulk value.

This work was supported by NYSTAR and NSF IGERT program.
C.1.00114 Quantum conductance of carbon nanotube at finite temperature: effect of electron-phonon interactions

NARJES GORBIZADEH, Tohoku University, AMIR A. FARAJIAN, Wright State University, YOSHIIYUKI KAWAZOE, Tohoku University — Effect of inelastic electron-phonon interaction is studied on electronic transport of semiconducting carbon chains and carbon nanotubes. Absorption and emission of individual phonon modes are investigated as well as collective modes in order to reveal the nature of the interactions and the role of vibrations in quantum transport at finite temperature. The conductance in this study is calculated using non-equilibrium Green’s function formalism combined with a tight-binding Hamiltonian description. The phonon spectrum is obtained from frozen-phonon approach and the electron-phonon interaction appears in the calculations as a coupling matrix determined by atom-displacements and phonon eigenvectors. Our results show that the effect of individual electron-phonon interaction on quantum conductance depends on temperature and energy of the phonon mode, regarding absorption and emission processes. The type of the phonon mode is in fact a determining part of the interactions. Decrease of conductance due to e-ph scattering is stronger when the process is scattering of electron out of in-plane phonons which make the in-plane C-C bonds of nanotube or chain vibrate with higher length. The effect of collective modes also suggests the temperature dependent nature of the conductance of a finite size carbon chain and nanotube.

C.1.00115 Detection of multiple tumor markers using ultra-long carbon nanotube devices

HYE-MI SO, DONG-WON PARK, BEOM SOO KIM, KI-JEONG KONG, GYOUNG-HO BUH, HYUNJU CHANG, JEONG-O LEE, Korea Research Institute of Chemical Technology, JING KONG, Massachusetts Institute of Technology — For the simultaneous detection of multiple tumor markers, we have fabricated ultra-long carbon nanotube sensors that can detect carcinoembryonic antigen (CEA) and prostate specific antigen (PSA), simultaneously. Ultra-long carbon nanotubes, several millimeters long, were grown by ethanal CVD, and fabricated as FET sensors by using conventional photolithography. To functionalize each segment of a single ultra-long nanotube device with multiple-tumor markers, we first functionalize the entire device with CDI-Tween 20 linking molecules, and then immobilized CEA and PSA antibodies using the micorfluidic channel. The electrical conductance from CEA-antibody functionalized and PSA-antibody functionalized segment of a ultra-long carbon nanotube device was monitored simultaneously with Ag/AgCl reference electrode as a liquid gate. We will discuss the advantages of long-nanotube device in detail.

C.1.00116 Low-temperature electronic transport in ferromagnetic cluster embedded carbon nanotubes

CATERINA SOLDANO, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, SWASTIK KAR, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, ROBERT VAJTAI, Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, SAIKAT TALAPATRA, Department of Physics, University of Southern Illinois at Carbondale, SAROJ NAYAK, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, PULICIKEL AJAYAN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — We present the electronic transport properties of ferromagnetic material embedded alumina template grown carbon nanotubes. Zero-field temperature dependence of the conductance in ferromagnetic cluster-embedded tubes (FM-MWNT) reveals a Lüttinger liquid type of behavior in the higher temperature region. Differential conductance measurements for discrete applied magnetic field show the appearance of field-dependent oscillations at low temperatures. The properties of the FM-MWNT were found to change permanently under the application of a magnetic field, indicating that the charge transport is sensitive to the relative magnetic orientations (random or aligned) of the nanoclusters. Those measurements suggest differences between charge transport in a Lüttinger liquid under the influence of "random" and "ferromagnetically aligned" impurities.

C.1.00117 Local-gated single-walled carbon nanotube field effect transistors assembled by AC dielectrophoresis

PAUL STOKES, SAIFUL I. KHONDATER, NANOSCIENCE TECHNOLOGY CENTER & DEPARTMENT OF PHYSICS, UNIVERSITY OF CENTRAL FLORIDA, ORLANDO, FL TEAM — Carbon nanotube field effect transistors (CNT-FETs) have displayed exceptional electrical properties that are superior to the traditional silicon MOSFET. Directed assembly of individually addressable CNT-FETs at selected positions of the circuit with high throughput needs to be demonstrated for future integrated circuits. Here, we present a simple and scalable technique for the fabrication of CMOS compatible & local gated CNT-FETs. The approach is based on directed assembly of individual single-walled carbon nanotube from dichloroethane via AC dielectrophoresis (DEP) onto pre-patterned source and drain electrodes with a local Al gate in the middle. We find that both metallic and semiconducting nanotubes can be assembled and the centered aluminum gate does not affect the DEP assembly. We also show that the measured device performance such as subthreshold swing of local-gated semiconducting nanotube FET is superior compared to the global back gated device possibly due to channel controlled operation. Directed assembly of local gated CNT-FETs at selected position of the circuit via DEP pave the way for large scale fabrication of CMOS compatible nanoelectronic devices.

C.1.00118 Microwave Magnetolectric Coupling in Ferromagnetic-Piezoelectric Nanostructures

YU.J. PUKINSKY, M.I. BICHURIN, V.M. PETROV, A.V. FILIPPOV, S.V. BELY, Novgorod State Univ. Russia, G. SRINIVASAN, Oakland Univ., MI — A theory is presented on the effect of an external electric field on ferromagnetic resonance (FMR) spectra of nanobilayers, nanopillars and nanowires of ferrite and piezoelectrics on MgO or gadolinium gallium garnet substrates. Expressions have been obtained relating the FMR line shift to ME coupling constants. Estimates of ME coupling constants are given. With increasing substrate thickness, the theory predicts a decrease in the ME interaction due to the clamping effect. The strongest ME coupling is expected for ferrite nanopillars in a piezoelectric matrix when the pillar height is large compared to substrate thickness. Numerical estimations are obtained for nanostructures of nickel ferrite and PZT or PMN-PT, yttrium iron garnet and PZT or PMN-PT on MgO or gadolinium gallium garnet substrates. The theory is useful for measurements of ME constants and for the design and analysis of electrically controlled high frequency devices.

C.1.00119 Enhancement of Magnetolectric Effect in Ferromagnetic-Piezoelectric Nanostructures at Electromechanical Resonance

A.V. KOZIN, M.I. BICHURIN, YU.J. PUKINSKY, V.M. PETROV, Novgorod State Univ. Russia, G. SRINIVASAN, Oakland Univ., MI — A theoretical model is presented for giant magnetolectric (ME) coupling in nanobilayers, nanopillars and nanowires of ferrite and piezoelectrics on MgO substrates or templates in the electromechanical resonance region (EMR). We take into account clamping effect of the substrate in determining the ME voltage coefficient. ME coefficients are obtained from known material parameters (piezoelectric modules, magnetostiction, stiffness, geometrics) using the solution of the elastodynamic and electrostatic equations. With increasing substrate thickness the theory predicts a shift in the resonance frequency along with a decrease in the ME interaction due to the clamping effect. The strongest interactions are expected for ferrite nanopillars in a piezoelectric matrix when the pillar height is large compared to substrate thickness. As an example, the ME voltage coefficients are estimated for nanostructures based on nickel and cobalt ferrites and piezoelectric PZT and PMN-PT. Although the estimates here are based on bulk material parameters, it can easily be refined to take into account parameters for nanosized components.

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1 Supported by grants from NSF, Russian Foundation for Basic Research and Russian Ministry of Education and Science.

2 Supported by grants from NSF, Russian Foundation for Basic Research and Russian Ministry of Education and Science.
C1.00120 Electronic Properties of XB₆ rods: a theoretical study¹, GUANGPING LI, JING LU, R.F. SABIRIANOV, W.N. MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, C.L. CHEUNG, X.C. ZENG, Department of Chemistry, University of Nebraska - Lincoln, Lincoln, NE 68588 — Metal hexaborides have varieties of interesting properties and are utilized frequently in technological applications: LaB₆ has low work function (WF=2.6 eV), and is used as electron emitter. Experiments indicated LaB₆ nanorods generate stronger electric current than in the bulk case. We focus on the electronic structure of quasi-1D XB₆ nanorods (X = Si, Ca, Sr, Y, Ba, and most of the rare earth elements) with various widths and breadths for studying the relationship between WF and rod shape by using density functional theory with many-body and relativistic effect included. Then the electronic structure properties such as Fermi energy and electrostatic potentials can be calculated to deduce the work function. Cluster model with several cross section areas is used to investigate the size dependence of ionization potential which is found to decrease with the increasing number of unit cells: 3.3 eV for 1-cell and 2.7 eV for 6-cell cluster. The trend is in reasonable agreement with the experimental studies.

¹This work is supported by Nebraska Research Initiative.

C1.00121 Optical Determination of the Flexural Rigidity of Carbon Nanotube Ensembles¹, PRABHAKAR BANDARU, CHUNING NI, CHRISTIAN DECK, Materials Science, UC, San Diego — We demonstrate two simple and consistent optical methods for quantitatively determining the flexural rigidity (EI, where E is the elastic modulus and I the moment of inertia), a quantity of practical importance in determining the deflection and buckling characteristics of carbon nanotubes (CNTs). This is done through monitoring the deflection of patterned arrays of CNTs subject to fluid flow. In addition to mechanical characterization of filamentous nanostuctures, the implications of our work extend to the monitoring of nanoscale fluid flows, for tactile and shear force sensors and the characterization of the mechano-sensor response of cilia in physiology.

¹We acknowledge financial support from the NSF and the Office of Naval Research.

C1.00122 ABSTRACT WITHDRAWN —

C1.00123 Crystallization of titania nanotubes powders synthesized by anodization in chloride ions containing solutions, EUGEN PANAITESCU, LATIKA MENON, Physics Department, Northeastern University — Titanium oxide nanotubes show good promise in solar energy harvesting for photovoltaic cells and photocatalysis. Pristine anodic titania nanotubes are amorphous, and annealing procedures are employed for their crystallization. We investigated the crystallization process of titania nanotubes powders - obtained by anodization of titanium foils in chloride ions containing solutions - by means of differential scanning calorimetry. We analyzed the influence of parameters such as annealing temperature, annealing time, and temperature scan rate on the phase transition, and on the crystalline properties of the final product. The crystalline powders have been characterized using XRD, RAMAN and diffuse reflectance measurements. SEM and TEM imaging has been employed for the investigation of structural properties before and after annealing, and optimal annealing conditions have been identified.

C1.00124 The size controlled structural and optical properties of ZnO nano-rod arrays, YANWEI CHEN, GUOLIANG YANG, Drexel University, QIAN QIAO, YICHUN LIU, Northeast Normal University — In comparison with zero dimensional (0D) nanostuctures, one-dimensional (1D) semiconducting nanostructures can facilitate more efficient carrier transport due to decreased grain boundaries, surface defects and disorder, and discontinuous interfaces. In order to utilize 1D ZnO nanostructures for optoelectronic nanodevices, it is essential to have detailed information about their size and other properties and to have the ability to tune these properties in the fabrication process. The application of the 1D nanostructures depends on this tenability. At present, it is still a challenge to fabricate well-controlled 1D ZnO nanostructures and to characterize their properties. We used convenient and flexible sol-gel and hydrothermal methods to synthesize 1D ZnO nanorods with diameters in the order of 10 to 20 nm. The crystalite size, morphology, the structural and optical properties could be well controlled by modulating the crystal nuclei quantity, the solution concentration and the reaction time. We obtained a strong ultraviolet exciton emission for the ZnO nanorods with a size about 10 nm, and also observed the size effect on the photoluminescence.

C1.00125 Linear optical response of (6,0) boron nitride nanotubes adsorbed with molecular hydrogen¹, N. NORBERTO ARZATE, RAUL A. VAZQUEZ-NAVA, Centro de Investigaciones en Optica, Mexico, JORGE E. MEJIA, Centro Universitario de los Lagos, Universidad de Guadalajara, Mexico — We performed a study of the molecular adsorption of hydrogen on BN nanotubes. We present ab initio calculations for the linear optical response of single wall zigzag BN(6,0) nanotubes as a function of the hydrogen adsorption on the exterior surface of the nanotube. The calculation of the linear optical response is performed by using density functional theory with the use of plane waves and pseudopotentials. We consider four different nanotube-structures adsorbed with different coverage of molecular hydrogen. We find optimized atomic coordinates for such structures and calculate binding energies for the molecule of hydrogen on the nanotube. After having the linear response of the considered structures, we have calculated their energy loss function spectra.

¹This work has been partly supported by CONACYT, Mexico, grants: SEP-2004-C01-48142 and SEP-2003-C02-12576, SEP-2005-C01-49678-F.

C1.00126 Magnetostrictive effects in a bilayer of PZT and magnetostriction-graded ferrite¹, G. SRINIVASAN, Oakland University, Rochester, MI, V.M. PETROV, Novgorod State University, Russia — Magnetostrictive (ME) effects in a piezoelectric-magnetostrictive composite are mediated by mechanical stresses. The effect, in particular, will be enhanced in the electromechanical resonance region (EMR) where the electronic subsystem shows resonance. We show here that further enhancement of the strength of ME interaction is possible with the use of magnetostriction-graded ferromagnet. A material with the grading axis perpendicular to the sample plane is considered. In this case, the thickness dependence of the piezomagnetic coefficients leads to additional bending strain, resulting in an increase in the EMR voltage. Estimates are provided for a bilayer of Zn-doped nickel ferrite and lead zirconate titanate, length 12 mm in length and 2 mm in thickness. The EMR voltage coefficient is predicted to increase by a factor of two compared to bilayers with homogeneous ferrite compositions.

¹Supported by grants from NSF and Russian Foundation for Basic Research.

C1.00127 Magnetoelectric properties of a bilayer of magnetostrictive and piezoelectric nanofilms- studies on substrate pinning effects¹, GOPALAN SRINIVASAN, Oakland Univ., V.M. PETROV, Novgorod State University, Russia — A model is presented for magnetoelectric (ME) effects in the electromechanical resonance region (EMR) for bilayers of magnetostrictive and piezoelectric films on a substrate. The clamping effect of the substrate has been considered in determining the ME voltage coefficient for longitudinal (or radial) and bending modes. The ME effect is predicted to be weak due to pinning and is dependent on the substrate volume. It is shown that the dependence of ME effect on the substrate thickness is much weaker for bending modes than for radial or longitudinal modes. For increasing volume of the substrate, the EMR frequency decreases dramatically. In the case of a rectangular nickel ferrite-PZT nanobilayer on an MgO substrate, the EMR frequency is predicted to be minimum when the substrate is clamped at one end.

¹Supported by grants from NSF and Russian Foundation for Basic Research.
C.1.00128 Theory of magnetoelectric coupling in magnetostrictive-piezoelectric bilayer at bending modes\textsuperscript{1}, A.V. FILIPPOV, N.A. FEDOTOV, M.I. BICHURIN, V.M. PETROV, Novgorod State Univ., Russia, G. SRINIVASAN, Oakland Univ., MI, CE-WEN NAN, Tsinghua Univ., China — Magnetoelastic (ME) couplings in bilayers of magnetostrictive and piezoelectric phases result from mechanical deformation. Reports to-date focused mainly on enhancement of the ME effect in the electromechanical resonance (EMR) corresponding to radial modes. Recent investigations, however, showed a similar enhancement and a giant ME effect for the bending modes of EMR in ferromagnetic-piezoelectric layered structures. Such bending modes are expected to occur at a much smaller frequencies than radial modes. Here we provide the frequency dependence for longitudinal and transverse ME voltage coefficients using a simultaneous solution of electrostatic, magnetostrictive and elastodynamics equations. The resonance ME effect in a bilayer is shown to be strong, depending on boundary conditions. A giant ME coefficient for bending modes is predicted for a bilayer fixed at one end and free at the other. The ME voltage coefficients are estimated from known material parameters (piezoelectric coupling, magnetostriction, elastic constants, etc.) and are compared with data. 

\textsuperscript{1}Supported by grants from NSF, Russian Foundation for Basic Research and Russian Ministry of Education and Science.

C.1.00129 Photo-formation of Gold Nanoparticles in Au(III)-chitosan-silica aerogels: Dependence on Wavelength and Duration of Exposure\textsuperscript{1}, NARAYANAN KUTHIRUMMAL, ADAM DEAN, RICHARD SMITH, ALEM TEKLU, College of Charleston — Porous transparent monoliths of Au(III)-chitosan-silica aerogels have been exposed to UV light (320 nm and 207 nm). The photoacoustic spectra of UV-exposed sample revealed a new peak around 526 nm, which corresponded to the plasmon resonance band of gold nanoparticles. Scanning electron microscopic and elemental analysis revealed the presence of gold particles. The plasmon peak is found to shift significantly to the blue side upon irradiating the sample for a longer time interval. It is possible that the nanoparticle heats a bit and could anneal its surface surrounding leading to a slight reduction in size. Electron microscopic observations show morphological changes upon increasing the UV exposure time. A relative larger shift observed upon exposing the sample to 200 nm light. Based on the present results, it is concluded that the gold particle size can be altered by changing the duration of light exposure or by using a different wavelength.

\textsuperscript{1}This work was supported by the Nanotechnology Undergraduate Education (NUE) program of the National Science Foundation (Award No.EEC-0634142).

C.1.00130 Elasticity and mechanical properties of nanostructured carbon\textsuperscript{1}, MARIA FYTA, Department of Physics, Harvard University, IOANNIS REMEDIARIS, Department of Materials Science and Technology University of Crete, Heraklion, Crete, Greece, PANTELIS KELIRES, Department of Mechanical Engineering and Materials Science and Technology, Cyprus University of Technology, Limassol, Cyprus — We present a theoretical study of nanostructured carbon, emphasizing on diamond nanocomposites. These are materials that consist of diamond nanocrystals surrounded by a dense amorphous carbon matrix, in a highly stable configuration. We study the properties of such materials by employing a combination of tight-binding molecular-dynamics and empirical-potential Monte-Carlo simulations. We aim to investigate the role of the sp\textsuperscript{2} component and the grain size on the mechanical properties of these structures. We calculate the rigidity of these materials and their elastic recovery under hydrostatic pressure, and find them to be considerably high compared to those of dense single-phase amorphous carbon. We find that the inter-grain fracture of these materials under shear and tensile load on these materials occurs at the weakly bonded sp\textsuperscript{3} sites in the amorphous matrix.

\textsuperscript{1}Work done at Physics Department, University of Crete, Heraklion, Crete, Greece.

C.1.00131 Thermal conductivity of Cu/carbon nanotube composite films, JUNG JOON YOO, Korea Advanced Institute of Science and Technology, HO-KI LYEO, JAE YONG SONG, SUNGJUN LEE, Korea Research Institute of Standards and Science, JIN YU, Korea Advanced Institute of Science and Technology — We report the thermal conductivity of Cu/carbon nanotube (CNT) composite films measured by time-domain thermoreflectance, an optical pump-probe method, which measures the time-evolution of temperature change. The thermal and electrical conductivities of sputter-deposited Cu, electroplated nanocrystalline (nc) Cu, and Cu/CNT composite films are measured with a varying content (0 ∼ 2 wt%) of CNT in Cu matrix. Both conductivities of nc-Cu films grown on a seed layer of sputtered Cu decrease significantly compared to those of bulk Cu. The thermal conductivity of Cu/CNT composite films made of nc-Cu and randomly oriented CNTs decreases further with the increase of CNT in the films. With the increasing amount of CNT, we also measure the decreasing thermal conductance of interface between Cu/CNT composite film and Al layer that is used as a transducer for the measurement. We will discuss the relations between CNT content and the measured reduction of thermal conductivity and conductance, depending upon the microstructure and impurities of composite films.

C.1.00132 Percolation Studies of Metal-insulator Composites at Microwave Frequencies\textsuperscript{1}, KELLY MARTIN, JEREMY CARDELLINO, EARNIE JOHNSON, NICHOLAS MISKOVSKY, GARY WEISEL, DARIN ZIMMERMANN, The Pennsylvania State University, Altoona College, JUNKUN MA, Southeastern Louisiana University — We present a systematic study of the effective dc conductivity (σ_{eff}), complex permittivity (\varepsilon_{eff}) and complex permeability (\mu_{eff}) at microwave frequencies, of metal-insulator mixtures up to and beyond the critical volume fraction (\phi_{c}) for conductive percolation. Samples made with varying concentrations of Teflon and micron-sized metallic inclusions of copper, silver, cobalt, and tungsten were subjected to separated microwave electric and magnetic fields of a 2.45 GHz, TM_{010} resonant cavity. Using cavity perturbation techniques, the real and imaginary components of \varepsilon_{eff} and \mu_{eff} were thus measured at room temperature. We observe the expected strong dependence of \sigma_{eff}, \varepsilon_{eff}, and \mu_{eff} on volume fraction \phi_{c} and analyze the results using Mclachlan’s Generalized Effective Medium (GEM) theory to extract \phi_{c} and the percolation exponents s and t.

\textsuperscript{1}This work is supported in part by a grant from the National Science Foundation (NSF/RUI: DMR-0406584), The Pennsylvania State University, and Altoona College.

C.1.00133 The electronic spectrum of a quasiperiodic potential: from the Hofstadter butterfly to the Fibonacci chain, GERARDO NAUMIS, Depto. de Fisica-Quimica, Instituto de Fisica, UNAM — We show that the electronic spectrum of a tight-binding Hamiltonian defined in a quasiperiodic chain with an on-site potential given by a Fibonacci sequence, can be obtained as a superposition of Harper potentials. Since the spectrum of the Harper equation as a function of the magnetic flux is a fractal set, known as Hofstadter butterfly, here we show that is possible to follow the transformation of the butterfly to a new one that contains the Fibonacci potential and related approximants. As a result, the equation in reciprocal space for the Fibonacci case has the form of a chain with long range interaction between Fourier components. Then we explore the transformation between both spectra, and specially the origin of energy gaps due to the analytical calculation of the components in reciprocal space of the related potentials. As an application, we calculate the correlator of each potential, which allows to obtain some of the localization properties.
C1.00134 Ab initio studies of molecular physisorption on graphene¹, DAVID CAREY, DANIEL HENWOOD, University of Surrey — Ab initio studies of the hydrogen and oxygen molecular physisorption have been made on a graphene using both the local density approximation (LDA) and generalized gradient approximation (GGA) PW91 functionals. Binding energies and optimal molecular separations for different graphene lattice sites have been calculated. It was found that the most stable binding energy is for the hydrogen molecule to lie at a hexagon mid-point with a binding energy of 93 meV as calculated for a 96 carbon atom graphene layer using the LDA functional. Lower values of hydrogen molecular binding were found with the GGA functional. [1] Analysis of the charge distribution showed little charge transfer between the molecule and graphene sheet. Oxygen physisorption is shown to be significantly stronger than hydrogen physisorption with calculations using the LDA functional showing binding energies of 280 meV. [1] Daniel Henwood and J David Carey, Phys. Rev. B 75, 245413 (2007).

¹Funding from the EPSRC (UK) is gratefully acknowledged.

C1.00135 The Transport of Graphene in a Parallel Field, ADAM FRIEDMAN, ANISH MOKASHI, LATIKA MENON, Northeastern University Dept. of Physics — The recent discovery of graphene and its remarkable properties has generated an enormous amount of research and has led some to contemplate it as a replacement for silicon in the next generation of computer chips. A large amount of theoretical work has been completed, but very little experimental work has been done to verify the theory. In particular, experiments have neglected the effect of a magnetic field applied parallel to the 2-D surface plane. Theory [1] has predicted that this orientation of magnetic field will split the spectra of particles and holes, which will then interact with each other through attractive Coulomb forces, driving a metal to gapped insulator transition. We will report the results of experimental studies of the transport in graphene at a parallel magnetic field at low temperatures. [1] I. L. Aleiner, D. E. Kharzeev, and A. M. Tsvelik, arXiv:cond-mat/0708.0394

C1.00136 Numerical study of electronic transport in a graphene superlattice, DI WU, WEI-QIANG CHEN, FU-CUN ZHANG, Department of Physics and the Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China — Using tight-binding model, We calculate the transport properties of charge carriers through graphene superlattices consisting of monolayer or bilayer graphene with an applied external potential barrier. Emphasis is placed on inter-valley scattering between two inequivalent Dirac cones in our systems. It is shown that transmission probabilities for two kinds of graphene structure exhibit different features due to distinct intrinsic properties of charge carriers in these superlattices. The co-existence of inter-valley and intra-valley scattering in the monolayer lattice declines the phenomenon of perfect transmission predicted by Klein paradox.

C1.00137 Magnetic edge states in graphene, SUNGHUN PARK, H.-S. SIM, Korea Advanced Institute of Science and Technology — We theoretically study the magnetic edge states of the Dirac fermions in graphene, formed along the boundary between the two domains in a spatially nonuniform magnetic field, Bᵢ in one domain and Bᵣ in the other domain, in the quantum Hall regime. The energy spectra of the magnetic edge states depend on whether Bᵢ is parallel or antiparallel to Bᵣ. For the parallel case, the n=0 magnetic edge states are dispersionless, while they split into electron-like and hole-like levels for the antiparallel case. Here, n is the graphene Landau level index. These features are attributed to the coupling between the pseudo-spin of the magnetic edge states and the direction of the external magnetic field. We also study the modification of the energy spectra when the finite Zeeman splitting or an electrostatic step-like potential is considered. An Aharonov-Bohm interferometry, which can identify the existence of the magnetic edge states, is suggested for experimental study.

C1.00138 Organic-inorganic Schottky diode based on few layers of graphene, MARIA ABREU, IDALIA RAMOS, NICHOLAS PINTO, University of Puerto Rico- Humacao — A Schottky diode was fabricated using several layers of graphene and a n-doped semiconductor and electrically characterized. The diode current-voltage characteristics show that it is forward biased in the first quadrant and reverse biased in the third. The diode turn on voltage is weakly dependent on temperature and increases slightly upon lowering the temperature. The diode rectification ratio is parallel or antiparallel to Bᵢ. For the parallel case, the n=0 magnetic edge states are dispersionless, while they split into electron-like and hole-like levels for the antiparallel case. Here, n is the graphene Landau level index. These features are attributed to the coupling between the pseudo-spin of the magnetic edge states and the direction of the external magnetic field. We also study the modification of the energy spectra when the finite Zeeman splitting or an electrostatic step-like potential is considered. An Aharonov-Bohm interferometry, which can identify the existence of the magnetic edge states, is suggested for experimental study.

C1.00139 Ferromagnet proximity effect in graphene bilayer, YURIY SEMENOV, North Carolina State University, JOHN ZAVADA, U.S. Army Research Office, KI WOOK KIM, North Carolina State University — A well-known effect of ferromagnet proximity in metallic thin film results in the giant magneto-resistance (GMR). In case of graphene monolayer, the effect of dielectric ferromagnet layer (DFL) proximity leads to formation of spin-dependent electron potential and electron spin rotation in effective exchange field. We theoretically consider the ferromagnet proximity effect in a graphene bilayer (GBL), where bottom and top layers are affected by arbitrary oriented DFL. Our calculations show a drastic reconstruction of energy bands structure with the top DFL magnetization rotation compared to the bottom one, which is assumed to be fixed by an antiferromagnetic substrate. If the top and bottom magnetic moments are parallel and equal, we obtain a simple spin split gapless band structure. As soon as symmetry between the top and the bottom GBL is broken by rotation of top DFL magnetization, the gap is opening; it reaches the magnitude of exchange field at antiparallel configuration. Calculated conductivity of GBL strongly depends on magnetic configuration demonstrating efficiency of the new mechanism of GMR.

²This work was supported in part by US ARO and the FCRP on FENA.

C1.00140 The Magnetic effect of Nonmagnetic Defect on Graphene, HIDEKI KUMAZAKI, DAI HIRASHIMA, Nagoya University — We study the effect of a nonmagnetic defect on magnetism of graphene. Magnetism in carbon-based materials has been a controversial problem. Apart from magnetic defects, the nonmagnetic-defect-induced mechanism is the most probable mechanism in those materials. In this presentation, we focus on vacancy-induced magnetism. Electrons in graphene can be described with a half-filled Hubbard model on a honeycomb lattice. We then introduce a vacancy as a short-range strong scattering potential on a lattice point. Resorting to a mean field approximation and diagonalizing the approximated Hamiltonian, we can determine the electron number and spin densities at each lattice point. We then find that a vacancy induces short-range ferrimagnetic order around itself. This order is caused by a quasilocalized vacancy state induced by a strong potential. In cases with extended vacancies, the moment formation depends on the geometrical structure and the difference in the numbers of vacancies on two sublattices. The magnetic moment is necessarily induced when the number of vacancies on one sublattice is unequal to that on the other sublattice, in accordance with Lieb’s theorem. We further discuss the possible magnetic moment formation on realistic edges in graphene.

C1.00141 Pseudospin Magnetism in Graphene¹, HONGKI MIN, The University of Texas at Austin, GIOVANNI BORGHI, MARCO POLINI, NEST-CNR-INFN and Scuola Normale Superiore, Italy, ALLAN H. MACDONALD, The University of Texas at Austin — We predict that neutral graphene bilayers are pseudospin magnets in which the charge density-contribution from each valley and spin spontaneously shifts to one of the two layers. The band structure of this system is characterized by a momentum-space vortex which is responsible for unusual competition between band and kinetic energies leading to symmetry breaking in the vortex core. We discuss the possibility of realizing a pseudospin version of ferromagnetic metal spintronics in graphene bilayers based on hysteresis associated with this broken symmetry.

¹Work at UT Austin was supported by the Welch Foundation, NRI-SWAN, ARO, and DOE.
C1.00142 Electron-electron and spin-orbit interactions in armchair graphene ribbons1. MAHDI ZAREA, NANCY SANDLER, Ohio University — The effects of intrinsic spin-orbit and Coulomb interactions on low-energy properties of finite width graphene armchair ribbons are studied by means of a Dirac Hamiltonian. It is shown that metallic states subist in the presence of intrinsic spin-orbit interactions as spin-filtered edge states, in contrast with the insulating behavior predicted for graphene planes. A charge-gap opens due to Coulomb interactions in neutral nanotubes, that vanishes as $D \sim 1/W$, with a gapless spin sector. Weak intrinsic spin-orbit interactions do not change the insulating behavior. Explictic expressions for the width-dependent gap and various correlation functions are presented.

1Ohio University postdoctoral fellowship and NSF DMR 0710581

C1.00143 Electrical modulation in Graphene based devices1. HASSAN RAZA, EDWIN KAN, School of Electrical and Computer Engineering, Cornell University Ithaca NY 14853 — Graphene due to its unique dispersion has attracted great attention lately. In a nanobrion form, it can result in unique ‘bulk like’ states for armchair and edge states for zigzag nanoribbon. Both can be manipulated by an applied bias in the width direction and can result in interesting device concepts. Furthermore, the edge states can be engineered by modifying the edge termination, although atomic-precision is likely required. Moreover, a bandgap can be introduced in a bilayer using an electric field in the bilayer direction. This bandgap opening critically depends on the numbers of graphene layers. Motivated by this rich physics in one and two dimensional graphene structures, we present different bandstructure calculations of nanoribbons and multilayers of graphene. We extract important dispersion parameters from the above calculations. We further study the effect of electric field on these structures. Finally, we present the substrate effect on the electronic structure of graphene layers. We conclude by presenting transport calculations through nanoribbons in longitudinal direction with gate electric field in the width direction.

The work is supported by National Science Foundation (NSF) and by Nanoelectronics Research Institute (NRI) through Center for Nanoscale Systems (CNS) at Cornell University.

C1.00144 Spin channels in functionalized graphene nanoribbons, GIOVANNI CANTELE, CNR-INFM and University of Napoli “Federico II”, YOUNG-SU LEE, Korean Institute of Science and Technology, DOMENICO NINO, University of Napoli “Federico II”, NICOLA MARZARI, Massachusetts Institute of Technology — Graphene nanoribbons have attracted lot of interest, due to high potentiality in technological applications, mostly in graphene-based nanoelectronics. Electronic and transport properties may strongly be influenced by the crystallographic orientation as well as by the presence of defects and different chemical functionalizations. Among the possible edges, the zigzag ones deserve special attention, because it has been shown that magnetic ordering is obtained in the ground state, so as half-metallicity and spin-filtering behavior could in principle be observed under suitable experimental conditions. Here we show how the chemistry of the ribbon edge and surface may strongly affect the transport properties. Quantum conductance is calculated, with ab-initio accuracy, by combining a maximally localized Wannier function approach and the Landauer formula. We show that proper functionalization of the edges may strongly modify the electronic properties. Chemical species adsorbed on the nanoribbon surface can, on the other hand, significantly affect the spin channels, giving rise in some cases to an almost perfect spin-filtering behavior.

C1.00145 Ab initio study of alkali metal adsorption on various forms of graphene nanoribbons . SEON-MYEONG CHOI, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — Electronic and magnetic properties of graphene nanoribbons (GNRs) are very unique depending on their edge shape. While many theoretical studies of GNRs show such intriguing features, clear experimental proofs of atomic edges and their effect on electronic structures have not been explicitly demonstrated. One of the issues is the difficulty of identifying GNRs edges. In this study, we calculated the adsorption energy of alkali metal atoms on various forms of GNRs using the pseudopotential density-functional method. We present the distribution of adsorbed atoms on armchair- and zigzag-edged GNRs using the calculated adsorption energy. This approach can help classify the edge of GNRs from the distribution of adsorbed atoms.

C1.00146 Electronic structure and bonding properties of hydrogen on K(2x2)/Graphene1. CÉSAR ACOSTA, JORGE ALEJANDRO TAPIA, Facultad de Ingeniería, Universidad Autónoma de Yucatán, ROMEO DE COSS, Departamento de Física Aplicada, Cinvestav-Mérida — The effect of the adsorption of hydrogen atom on the electronic properties of K(2x2)/graphene system, are studied by means of first-principles calculations. The results were obtained with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. The structural parameters, bonding properties, and electronic structure of the H atoms on K/graphene system are calculated by molecular dynamics. We find an important charge transfer from the substrate towards the H atomates. The strong H-C chemical bond produced a considerable deformation in the graphene layer. The bonding energy of hydrogen is larger for the K/graphene system than for the single layer of graphene. The present results suggest that the hydrogen adsorption on layered carbon systems could be stimulated by the pre-adsorption of simple metals.

1This research was supported by PRIORI-UADY under Grant No. FING-05-004 and Consejo Nacional de Ciencia y Tecnología (CONACYT-México) under Grant No. 43830-F.

C1.00147 Spontaneous Decay and Two-Qubit Entanglement in Ion-Doped Carbon Nanotubes2. IGOR BONDAREV, NC Central University, NATALIA NOGINOVA, Norfolk State University — We study theoretically surface electromagnetic phenomena, such as spontaneous decay and entanglement of two-level atoms (qubits) close to a carbon nanotube surface[1]. The research is motivated by the progress in growth of cm-long single-walled nanotubes[2], single atom encapsulation into nanotubes[3], and the need for nanomaterials with long quantum coherence lifetimes with ab-initio accuracy, by combining a maximally localized Wannier function approach and the Landauer formula. We show that proper functionalization of the single layer of graphene. The present results suggest that the hydrogen adsorption on layered carbon systems could be stimulated by the pre-adsorption of simple metals.

2Supported by NSF via grant No ECS-0631347.

C1.00148 Uptake and isosteric heats of gases adsorbed inside carbon nanotubes1. DANIEL ROBERTSON, SILVINA GATICA, Department of Physics, Howard University — We studied the properties of gases adsorbed in the interior of open-ended single wall carbon nanotubes for a wide range of pressures and temperatures from tens to hundreds of Kelvin. The gases studied are Argon, Methane, Hydrogen and Helium in a classical regime. Using the method of Grand Canonical Monte Carlo Simulations we computed the adsorption isotherms, the isosteric heat of adsorption and the configurations at different T,P values. The thresholds values of the pressure and maximum uptake were calculated as a function of the temperature. At the lower temperatures the adsorption of atoms on the axis of the tube is observed as a discontinuous step in the isotherms.

1This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
C1.00149 Acetylene-Boosted Growth of Vertically Aligned SWNTs by Alcohol CCVD Method1, RONG XIAO, JUN OKAWA, ERIK EINARSSON, YUHEI MIYAIUCHI, SHICGO MARUYAMA, Department of Mechanical Engineering, The University of Tokyo, Japan — We present an interesting growth boost of vertically aligned SWNTs achieved by introducing a very small amount of acetylene into the conventional Alcohol Catalytic CVD (ACVD) system. This acetylene assisted ACCVD, as investigated in situ by optical absorption, not only provides us a way to enhance the SWNT growth rate by an order of magnitude, but also confirms that 0.1% of acetylene can reach the same activity as ethanol. Considering that acetylene is one of the products of thermal decomposition of ethanol at growth temperature, we might consider the chemical pathway from SWNTs via acetylene besides the direct pathway from ethanol. A no-flow ACCVD condition fully utilizes this decomposed acetylene as the growth promoter. Since this highly efficient growth through acetylene is only observed with sufficient accompanying ethanol, the critical roles of ethanol and acetylene are discussed.

1The present work was supported in part through the 21st Century COE program, “Mechanical Systems Innovation,” by the Ministry of Education, Culture, Sports, Science and Technology.

C1.00150 The evolution of helical forms in nanotube and nanofiber growth: Thermodynamic Model and Experiment, PRABHAKAR BANDARU, Materials Science, UC, San Diego, APPARAO RAO, Department of Physics, Clemson University — Several models, none of them completely satisfactory, have been proposed to understand the synthesis of nanotubes and nanocoils. In this presentation, we first briefly review the models in vogue and point out their shortcomings. Second, we introduce a thermodynamic model, based on exclusion volume principles, common in chemical and biological systems that could potentially explain coiling in nanostructures. Here, the observation of helices and coils in nano-tube/-fiber syntheses is explained on the basis of the interactions between specific catalyst particles and the growing nanostructure. Third, we make specific predictions for the optimal growth of nano-coils/-helices with the hope that these could be used as a guide for rational synthesis. Finally, our own experimental results conforming to the above model, on the role of Indium catalyst particles and local CVD reactor temperature in influencing the coil pitch in coiled nanostructures, will be presented.

C1.00151 Electroluminescence of a ZnS-based powder phosphor1, SO YEON JUN, Hankuk Univ. Foreign Studies, JIN-YOUNG KIM, Sungkyunkwan Univ., SANG HYEUN PARK, Samsung Adv. Inst. Technol., SEGY YU, Hankuk Univ. Foreign Studies — Electroluminescence (EL) and photoluminescence (PL) spectra of carbon nanotube (CNT) incorporated ZnS:Cu,Al inorganic powder phosphors under an AC voltage were analyzed by comparing with bare ZnS:Cu,Al powder. The spectra was obtained at room temperature with a He-Cd laser and a single grating monochrometer. By varying the frequency of the applied ac voltage, the PL and EL spectra yield distinct difference in the peak position, width, and intensity of the luminescence. As the concentration of CNTs were increased, the separation between the two luminescence peaks, which were analyzed by the Gaussian fitting, shrank. However, the spectra showed little different behavior for the voltage variation at fixed frequency. The underlying mechanism for this frequency dependence on CNT incorporation and EL performance enhancement will be mentioned in this poster.

1This work was supported by the Korea Research Foundation Grant. (KRF-2006-331-C00113)

C1.00152 Oscillatory Behavior of a Double Wall Carbon Nanotube Near an Infinite Surface2, ADRIAN POPESCU, LILIA WOODS, University of South Florida, IGOR BONDAREV, North Carolina Central University — Theoretical calculations of a double wall carbon nanotube oscillator with its axial direction perpendicular to an infinite surface are presented. The model for this work is based on the continuum approach of the pair-wise Lennard-Jones type of interaction in the double wall nanotube and between the nanotube and the surface. We investigate the oscillation frequency as a function of the distance between the nanotube and the surface, the length of the nanotube, and the magnitude of the initial excitation. Our calculations show that the oscillatory behavior is in the GHz region and it can be changed significantly by these factors. Based on these results, we suggest that the carbon nanotube oscillator can be used as a scanning device for surfaces in a similar manner as an atomic force microscope tip.

2Supported by DOE (DE-FG02-06ER46297).

C1.00153 Influence of surfactant concentration on the absorption and emission of light in single-wall carbon nanotubes, CRISTIANO FANTINI, Centro de Desenvolvimento da Tecnologia Nuclear — Optical absorption and photoluminescence have been largely used in the study and characterization of carbon nanotube samples, usually dispersed in aqueous solution wrapped with some surfactant. In this work we present a systematic investigation about the influence of the surfactant on the absorption and emission of light by carbon nanotubes. Carbon nanotubes dispersed in solution at different concentrations and wrapped with some different surfactant such as sodium dodecyl sulfate, sodium cholate, sodium dodecyl benzenesulfonate and segments of DNA were used in the experiments. Optical absorption and photoluminescence spectra were measured and the effects of both the kind of surfactant and the nanotube and surfactant concentrations on the photoluminescence efficiency were investigated. By comparing the intensities of absorption and emission it is possible to obtain the best nanotube and surfactant concentration for a higher efficiency in the emission of light. Changes in the absorption and emission energies are observed due to the environment screening on the exciton binding energies. Finally, we determine the structural assignment of the nanotubes and compare the dependence of the photoluminescence efficiency as a function of the surfactant and nanotube concentrations for different nanotube chiralities in the samples.

C1.00154 Theory of superplasticity and atomic relaxation in nanotubes and fullerenes, FENG DING, KUN JIAO, YU LIN, MS&MS Dept., Rice University, JIANYU HUANG, Center for Integrated Nanotechnologies, Sandia National Laboratories, BORIS I. YAKOBSON, MS&MS Dept., Rice University, YAKOBSON TEAM, JIANYU HUANG COLLABORATION — Plastic relaxation of carbon nanotubes under tension and at high temperature have been described in terms of dislocation theory and with atomistic computer simulations. Now we show how the glide of pentagon-heptagon defects and a particular type of their pseudo-climb [1], with the atoms directly breaking out of the lattice, work concurrently to maintain the tension and at high temperature have been described in terms of dislocation theory and with atomistic computer simulations. Finally, we make specific predictions for the optimal growth of nano-coils/-helices with the hope that these could be used as a guide for rational synthesis. Finally, our own experimental results conforming to the above model, on the role of Indium catalyst particles and local CVD reactor temperature in influencing the coil pitch in coiled nanostructures, will be presented.

1The present work was supported in part through the 21st Century COE program, “Mechanical Systems Innovation,” by the Ministry of Education, Culture, Sports, Science and Technology.
C1.00155 Carbon metal interactions and epitaxy in nanotube growth: Towards chirality-selected nanotube production, FENG DING, MS&MS Dept., Rice University, 6100 Main street, Houston TX 77005, PETER LARSSON, Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, SE-751 21 Uppsala, Sweden. J. ANDREAS LARSSON, Tyndall National Institute, University College Cork, Lee Maltings, Prospect Row, Cork, Ireland. RAJEEV AHUJA, Condensed Matter Theory Group, Department of Physics, Uppsala University, Box 530, SE-751 21 Uppsala, Sweden, ARNE ROSEN, KIM BOLTON, Physics Department, Göteborg University, SE-412 96, Göteborg, Sweden, BORIS I. YAKONSON, MS&MS Dept., Rice University, 6100 Main street, Houston TX 77005, FENG DING TEAM, GOTHEBURG UNIVERSITY COLLABORATION, UPPSALA COLLABORATION, UNIVERSITY COLLEGE CORK COLLABORATION — We report on formation of highly conductive SrTiO$_3$ and Technology (KAST) — We report on formation of highly conductive SrTiO$_3$ and Technology (KAST), TOSHIHIRO SHIMADA, TETSUYA HASEGAWA, Department of Chemistry, University of Tokyo / Kanagawa Academy of Science and Technology (KAST), YUTAKA FURUBAYASHI, YASUSHI HIROSE, Kanagawa Academy of Science, University of Tokyo / Kanagawa Academy of Science and Technology (KAST). Base on the optimized process 15 mm long CNT arrays were synthesized and preliminary data were obtained on spinning them into yarns.

C1.00156 Structural dependence of carbon nanotube orbital magnetic susceptibility: tight binding calculations, O. N. TORRENS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania — Recent ab initio calculations of the orbital magnetic susceptibility anisotropies in carbon nanotubes (CNTs) have shown large, systematic differences among zigzag CNTs of similar diameters [1]. We theoretically investigate the origin of these trends by applying the zone-folding method within the nearest-neighbor tight-binding approximation to all chiral and achiral semiconducting CNT species with diameters between 0.6 nm and 1.7 nm. Our results show qualitative agreement with the "mod 1" and "mod 2" trends of the ab initio theory and additionally distinguish between trigonal warping and curvature-related effects as physical reasons for the predicted species-dependent spread. Our calculations show (2n+m) patterns similar to those in a recent, experimentally-motivated "fan-out" diagram [2] and can be likewise fit to an analytical four-term chirality expansion. [1] Marques, M. A. L.; d’Avezac, M. & Mauri, F., Phys. Rev. B, 2006, 73, 120543 [2] Torrens, O. N.; Milkie, D. E.; Ban, H. Y.; Zheng, M.; Onoa, G. B.; Gerke, T. D. & Kikkawa, J. M., J. Am. Chem. Soc., 2007, 129, 252-253

C1.00157 Calculations of optical injection and coherent control in graphene, JULIEN RIOUX, JOHN E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto — We calculate injection spectra for one- and two-photon absorption in graphene, as well as optically injected currents from coherent control of one- and two-photon absorption in graphene, as well as optically injected currents from coherent control of 1 + 2 excitation. We compare ab initio pseudopotential calculations to analytical expressions of an effective tight-binding model expanded in $\vec{k}$ about the $K$ symmetric point. We find that the spectra from full-zone band structure calculations deviate from the simple model at energies above a few hundred meV’s.

C1.00158 Titanium Doped Carbon Nanotubes for Hydrogen Storage, JAKE FENNICK, JAMES LEWIS, West Virginia University — An efficient method of storing hydrogen is necessary before fuel cells can become practical. Previous computational results show that a single titanium atom adsorbed on the surface of a carbon nanotube can bind up to 4 hydrogen molecules. We pursue simulations of hydrogen packed between two titanium-doped carbon nanotubes. The highest percentage weight of storage and the manner in which these parallel nanotubes pack is of particular interest. Calculations are performed with the classical MD program GULP. After computation, automated analysis will choose the combination of parameters that results in the most efficient hydrogen storage for these titanium-doped carbon nanotube systems. [1] Yildirim, T.; Ciraci, S. Phys. Rev. Lett. 2005, 94, 175501.

C1.00159 Organic Light Emitting Diodes Using a Single Wall Nanotube Film Anode, EVAN DONOHUE, Dept. of Physics, University of Florida, KEN GRAHAM, Dept. of Chemistry, University of Florida, MATTHEW CRAPS, ZHUANGCHUN WU, Dept. of Physics, University of Florida, RYAN M. WALCZAK, JOHN R. REYNOLDS, Dept. of Chemistry, University of Florida, ANDREW G. RINZLER, Dept. of Physics, University of Delaware — To investigate single-wall carbon nanotube (SWNT) films as a replacement for indium tin oxide (ITO) as the anode in organic light emitting diodes (OLEDs), OLEDs constructed on SWNT films are compared to OLEDs on PEDOT:PSS/ITO. It is found that a single, simple polymer based device design of SWNT /poly[2-methoxy-5-(2’-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV)/Ca/Al can perform comparably with PEDOT:PSS/ITO OLEDs. For thick polymer layers of 300nm, both devices achieve a maximum light output of 700 cd/m$^2$ with efficiencies between 0.7-0.8 cd/A. The ITO device performance improves when a thinner MEH-PPV layer is used however variations in the SWNT film surface cause shorting if the MEH-PPV layer is substantially reduced in the SWNT anode devices. The advantages of a SWNT anode as well as the potential for future improvements will be discussed.

C1.00160 Extremely Long Multiwall Carbon Nanotube Arrays for Spinning Yarn, CHAMINDA JAYASINGHE, PRAVANAH SALUNKE, LUCY LEE, EMILY HEAD, Department of Chemical and Material Engineering, University of Cincinnati, Cincinnati, OH 45221-0012, NILANJAN MALLIK, YEHOEUNG YUN, Department of Mechanical Engineering, University of Cincinnati, Cincinnati, OH 45221-0072, CHANDRASHEKHAR PENDYALA, Department of chemical engineering, University of Louisville, Louisville, KY 40292, MARK J. SCHULZ, Department of Mechanical Engineering, University of Cincinnati, Cincinnati, OH 45221-0072, VESSELIN N. SHANOV, Department of Chemical and Material Engineering, University of Cincinnati, Cincinnati, OH 45221-0012 — Centimeter long Multiwall Carbon Nanotube (MWCNT) arrays have been grown by CVD from H$_2$-C$_2$H$_4$-$\text{H}_2$:Ar gas mixture at 750 °C in an Easy Tube furnace from First Nano Inc. The arrays were characterized by AFM, SEM, TEM and Raman spectroscopy. The diameter and chirality of the nanotubes were controllable by the choice of catalysts used. The full-length of 10 cm was the greatest impact on the nanotube diameter. The CVD growth has been optimized with respect to the length and the purity of theCNT. It was found that the CVD growth conditions affect dramatically the quality of the arrays. Base on the optimized process 15 mm long CNT arrays were synthesized and preliminary data were obtained on spinning them into yarns.

C1.00161 Formation of highly-conductive SrTiO$_3$-$\delta$ by pulsed laser deposition of TiO$_2$ on SrTiO$_3$ substrate, KUNITADA HATABAYASHI, Department of Chemistry, University of Tokyo, TARO HITOSUGI, Department of Chemistry, University of Tokyo / Kanagawa Academy of Science and Technology (KAST), YUTAKA FURUBAYASHI, YASUSHI HIROSE, Kanagawa Academy of Science and Technology (KAST), TOSHIHO SHIMADA, TETSUYA HASEGAWA, Department of Chemistry, University of Tokyo / Kanagawa Academy of Science and Technology (KAST) — We report on formation of highly conductive SrTiO$_3$-$\delta$ by pulsed laser deposition of TiO$_2$ on SrTiO$_3$ substrate under relatively reducing atmosphere. Anatase TiO$_2$ thin films were grown on SrTiO$_3$ (001) and (LaAlO$_3$)$_{0.3}$Sr$_2$AlTaO$_6$$_{0.7}$ (LSAT)(001), for comparison, by pulsed laser deposition under oxygen pressure of $P_{O_2}$ = 5x10$^{-8}$ Torr. In-situ RHEED (reflection high energy electron diffraction) measurements during film deposition revealed a clear streak pattern of 4K reconstruction, indicating growth of high quality anatase (001) films. Meanwhile, the anatase (001) films deposited on LSAT with thickness of >2 nm showed spotty RHEED patterns, indicating formation of oxygen-poor TiO$_2$-$\delta$. These facts lead us to a conclusion that oxygen atoms in SrTiO$_3$ substrate diffuse into anatase TiO$_2$ during the film growth process. In the TiO$_2$/SrTiO$_3$-$\delta$ heterostructure, we observed high mobility of 1x10$^4$ cm$^2$/Vs (5K) and Subnikov-de Haas oscillation (0.5K), proving formation of clean SrTiO$_3$-$\delta$ without structural deformation.
C1.00162 On the Electronic Structures of Ge Based Nanotubes.1 SOMILKUMAR RATHI, ASOK RAY, The University of Texas at Arlington — In the context of elucidating the properties of Ge-based nanotubes, we provide here a systematic ab initio study of the electronic and geometric structures of three different types of armchair silicon germanium nanotubes from (3, 3) to (11, 11) and compare them with the corresponding properties of Ge and GeC nanotubes. The finite cluster approach with dangling bonds terminated with hydrogen has been used. The theoretical formalism used is hybrid density functional theory incorporating HF exchange with DFT exchange-correlation functional. Full geometry and spin optimizations with unrestricted symmetry have been performed. A detailed comparison of the structures and stabilities of the nanotubes with dependence of the electronic band gaps on the respective tube diameters, energy density of states, dipole moments as well as Mulliken charge distributions have been investigated for all the tubes. Radial buckling of the tubes along with bond length variations is also studied and implications for band gap engineering will be discussed.

Work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525)

C1.00163 Wigner Function for a Quantum Wire with an Impurity, YI TANG, TOMAS MATERDEY, University of Massachusetts Boston — We present the Wigner function for a Gallium Arsenide (GaAs) quantum wire subjected to a magnetic field with an off-center donor impurity. The Wigner function is more sensitive to detecting changes than the variational wavefunction for smaller scale differences in a quantum wire with an impurity.

C1.00164 Computational Models for Catalyzed Growth of Si Nanowire. SEUNGHWA RYU, Department of Physics, Stanford University, WEI CAI, Department of Mechanical Engineering, Stanford University — We present molecular simulation models for the growth of silicon nanowires from gold catalyst particles. Because the number of atoms involve in this process is above 1000, it is infeasible to use ab initio models. Hence our first step is to develop an interatomic potential model for Au-Si using the modified embedded-atoms method (MEAM) framework. For the first time, we computed the Au-Si phase diagram entirely from the interatomic potential. The melting points are computed from free energy methods with uncertainties less than 1K. Molecular simulation of the interaction between the gold nanoparticle with the Si substrate and Si NW is presented.

C1.00165 Rapid Beam Shaping For Pulsed Laser Processing Using Tunable Acoustic Gradient Index Lenses, CRAIG ARNOLD, ALEXANDER MERMILLOD-BLONDIN, EUAN MCLEOD, Princeton University — Rapid shaping of an incident Gaussian laser beam enables spot-to-spot control over local material properties in pulsed and CW applications. Here we present a new device, the tunable acoustic gradient index (TAG) lens, which provides a rapid, high throughput alternative for spatially modifying incident beams and we discuss its effect on pulsed laser micromachining. The TAG lens is a resonant cylindrical cavity for acoustic radial standing waves that modulate the density and thereby create a gradient in index of refraction within the filling fluid. With CW illumination, a single driving frequency will produce a multiscale Bessel beam, or under multiple-frequency operation it can generate a superposition of Bessel beams, approximating any radially-symmetric pattern. When synchronizing a pulsed laser illumination to the lens, rapid switching between instantaneous patterns at frequencies as high as 100-1000 kHz is possible. The theory behind the operation of the lens, its speed, and applicability to pulsed laser processing will be presented.

C1.00166 Floating Tip Nanolithography YEHIAM PRIOR, KAIYIN ZHANG, ALEXANDER MILNER, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100, MICHAEL KARPOVSKI, Department of Physics, Tel Aviv University, Tel Aviv, Israel — We introduce a new mode of operation to standard atomic force microscopes, working under ambient conditions, for truly noncontact nanolithography. A phase-locked loop, based on tiny oscillations (<1 nm) of the cantilever at a frequency far from its mechanical resonance, is used to maintain the gap between the tip and the sample at a predetermined value of 1 - 4 nanometers continuously for long times without the tip ever touching the surface. In a geometry characteristic for Apertureless Scanning Near Field Optical Microscope, the tip is illuminated by a focused beam of a femtosecond laser (800 nm, 20 fsec, 100 mw ) for nano-patterning of the area under the tip. Under the laser irradiation the tip apex heats to a few hundred degrees as verified by a direct measurement of Raman line shifts, and the electromagnetric enhancement under the tip is used when the laser irradiates the actual tip apex. We demonstrate Floating Tip Nanolithography of two different types, both with lateral resolution of 10-20 nm. With a hot tip (the laser is not in contact with the surface) we thermally pattern the surface of a polymer film, and based on the electromagnetic field enhancement under the sharp tip we ablate narrow lines on a gold film. Future applications will be discussed.

C1.00167 Laser Desorption Ionization from Laser Induced Silicon Microcolumns: Surface Morphology and Chemistry, BENNETT N. WALKER, George Washington University, GUERMAN PASMANIK, Passat Inc., MD, AKOS VERTES, George Washington University — Nanomaterials and mesostructures, such as laser induced silicon microcolumn arrays (LISMA), offer new matrix-free platforms for laser desorption ionization (LDI) of biomolecules. The morphology and surface chemistry of LISMA depend on the processing environment and the laser parameters. Column diameters and lengths as well as periodicity, observed by AFM and SEM, depend on processing conditions (processing medium, laser pulse energy, pulse length and angle of incidence, etc.). Capillary waves at the molten silicon-processing liquid interface seem to initiate the development of LISMA structures. This is reflected by the correlation between the array morphology and the processing liquid density and interfacial tension. Ion yields from the various surfaces are dramatically affected by the pH of the processing environment, indicating a strong influence of the OH-terminated sites on the silicon surface. Ion generation from LISMA also significantly depends on the angle of the desorbing laser incidence, potentially suggesting energy coupling through an antenna array mechanism.

C1.00168 Internal Energy of Ions Produced by Laser Desorption/Ionization from Laser Induced Silicon Microcolumn Arrays, JESSICA A. STOOLEE, AKOS VERTES, George Washington University — Laser induced silicon microcolumn arrays (LISMA) were demonstrated as effective matrix-free laser desorption/ionization substrates for the mass spectrometry of biomolecules. Structure specific fragmentation of the produced ions primarily depends on their internal energy. To gain insight into the internal energy of ions laser desorbed from native LISMA and LISMA derivatized through sliane chemistry, the cations of eight benzyl-substituted benzylpyridinium salts were used as thermometer ions (TI). Survival yields of their unimolecular decomposition were determined and correlated to their internal energy through RRKM calculations. On both native and perfluorophenyl-derivatized surfaces, TIs showed no change in their internal energy over a wide range of laser fluence. While the survival yields for these preformed ions are stable, results on peptides indicate fluence dependent fragmentation. These results point to a different fragmentation mechanism for peptides mediated by hydrogen radicals formed through the recombination of protons, produced from residual solvents, and electrons, emitted from the silicon surface upon laser irradiation.
C1.00169 Nanoparticle Formation of Compound Materials, OMAR MUSAEV, VLADIMIR DUSEVICH, DAVID WIELICZKA, JERZY WROBEL, MICHAEL KRUGER, UMKC — UV pulsed laser radiation was applied to synthetic polycrystalline hydroxyapatite, the mineral that is the main component of bone. The process was carried out in deionized water. The ablated nanoparticles have been studied with Raman spectroscopy, TEM and XPS. According to transmission electron microscopy micrographs, the ablated particles were approximately spherical and had a size of ≈ 100 nm. Raman spectroscopic analysis indicated that particles had the same structure as the original crystal. XPS demonstrated that the surface chemical composition is similar to that of the original material. The advantage of this method in comparison with ablation in vacuum and gas is that due to the confinement conditions produced by the water, the composition of the ablated nanoparticles remains the same as the target material. Another advantage is in the simplicity of the method in comparison to both ablation in vacuum or low pressure gas and to chemical methods for nanoparticle synthesis.

1This work was partially supported by NSF.

C1.00170 Universal disorder in the microwave conductance spectra of doped silicon nanowire arrays, CLARK HIGHTRETE, MARK LEE, Sandia National Laboratories, AARON VALLETT, SARAH EICHFELD, JOAN REDWING, THERESA MAYER, Penn State University — Microwave conductance spectra of doped silicon nanowire (SiNW) arrays were measured from 0.1 to 50 GHz at temperatures between 4 K and 293 K. SiNWs were synthesized by VLS growth, assembled into arrays on co-planar waveguides and measured using microwave vector network analysis. The complex conductance of the arrays was found to increase with frequency at all temperatures as $\tilde{\sigma}^2$, with 0.25 < $s$ < 0.4, and to agree with the expected Kramers-Kronig relations. This AC conductance is consistent with behavior found universally in disordered systems. The likely cause is disorder from Si/SiO$_2$ interface states dominating the conduction due to the high surface-to-volume ratio of the nanowires. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. Penn State authors acknowledge partial support from NSF DMR-0213623 and NSF NRT ECCS-0609282.

1Also with Dept. of Physics & Astronomy, University of New Mexico

C1.00171 Size-dependent ionization of impurities in GaN nanowires, JOONAH YOON, ILAN SHALISH, School of engineering and applied sciences, Harvard University, L. R. RAM-MOHAN, Physics, Worcester Polytechnic Institute of Technology, VENKATESH NARAYANAMURTI, School of engineering and applied sciences, Harvard University. — The integration of nanowires into devices requires having dielectric materials in contact with the nanowire. Therefore understanding the effect of surrounding dielectric materials on properties of nanowires becomes quite relevant for the device integration of nanowires. In this work we present the effect of dielectric surroundings on electrical properties of gallium nitride nanowires. The conductivity of unintentionally n-doped gallium nitride nanowires is measured from 4.2 to 300 Kelvin. The ionization energies of impurities are extracted from the conductivity versus temperature measurements. These ionization energies are found to display a dependence on the radius of nanowires. This size dependence is explained by the self-energy correction due to the image charges formed at the surface of nanowires. We would like to emphasize this work is the first experimental work to report on the size-dependent ionization of impurities in nanowires

C1.00172 Highly electron-emitting states of boron-nitride nanotubes derived from the free-electron-like conduction band states, BINGCHAI YAN, Center for Advanced Study, Tsinghua University, Beijing, 100084, China, CHANGWON PARK, JISOO IHM, Department of Physics, Seoul National University, Seoul 143-747, Korea, GANG ZHOU, WENHUI DUAN, Center for Advanced Study, Tsinghua University, Beijing, 100084, China, NOEJUNG PARK, Department of Applied Physics, Dankook University, 44-1, Jukjeon-dong, Yongin-si, Gyeonggi-do, 448-701, Korea. — We investigate electronic structures and field emission properties of boron-nitride nanotubes (BNNTs) using the first-principles method and electronic dynamic simulations. To introduce a feasible transport channel we choose to dope alkali atoms to BNNTs. We show that the nearly free electron (NFE) state of a BNNT could shift down to the Fermi level, preserving the free-electron-like dispersion along the axial direction. Meanwhile the downshifted NFE state bears s-wave characters, which is necessary for an efficient electron field emission. Our dynamic simulations of emission current reveal that the BNNTs are much favorable for electron field emission, owing partially to the presence NFE states as well as low electron affinity. We suggest that a high-performance field emission devices could be fabricated using n-type doped BNNTs.

1Partly supported by JSPS-NSFC-KOSEF, A3 Foresight Program.

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C1.00176 Free standing carbon nanotubes growth on large-area by nanoimprint and plasma-enhanced chemical vapor deposition, WON SEOK CHANG, DAE-GEON CHOJ, JUN-HO CHUNG, KAB-SOO HUH, KIMM, NEMS TEAM — Among various synthesis methods for carbon nanotube growth, chemical vapor deposition (CVD) method has been widely used for various advantageous such as high quality, vertical alignment, controlled diameter and length of nanotubes and so on. Especially, vertically aligned multi-wall carbon nanotube could be grown using plasma-enhanced chemical vapor deposition (PECVD). In this paper, we presented growth of free standing carbon nanotubes by PECVD for the fabrication of nano-electrode. For the growth of nanotubes on the large area 50 mm x 50 mm, catalyst dots were formed by nanoimprint and lift-off process. The synthesis of carbon nanotube requires a metal catalyst layer, etchant gas, and a carbon source. Ammonia (NH$_3$) and acetylene (C$_2$H$_2$) were used as the etchant gas and carbon source, respectively. And iron (Fe) of catalyst metal was deposited on silicon wafer substrates. To form Fe nano dots with diameter of 150 nm and thickness of 50 nm, nano holes patterned imprint resin was used for lift-off process. Carbon nanotubes were grown on pretreated substrates at approximately 30% C$_2$H$_2$:NH$_3$ flow ratios for 40 min.

C1.00177 Ab initio calculation of intrinsic spin-Hall effect in graphene nanostructures, BIN WANG, JIAN WANG, Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China, HONG GUO, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, PQ, Canada H3A 2T8 — We report a theoretical analysis of intrinsic spin-Hall effect in a four-probe graphene nanostructure in the absence of spin orbit interaction and magnetic field. The nanostructure consists of a finite size graphene sheet connected to the outside world by two zigzag graphene nano-ribbons (ZGNR) and two armchair graphene nano-ribbons (AGNR), forming a cross- shaped two-dimensional device. Due to edge states induced magnetism at ZGNR boundaries, our result suggests that a pure spin-current without an accompanying charge current, is intrinsically induced giving rise to a spin-Hall effect. We have calculated the spin-Hall conductance by an atomic first principles method where density functional theory is carried out within the Keldysh nonequilibrium Green’s function framework.
C1.00178 Electronic properties of bilayer graphene ribbons with Bernal stacking in a strong magnetic field. YUAN-CHENG HUANG, Center for General Education, Kao Yuan University, CHENG-PENG CHANG, Center for General Education, Tainan University of, MING-FA LIN, Department of Physics, National Cheng Kung University — We employ the Peierl coupling tight-binding method to study magneto-electronic properties of bilayer graphene ribbons with Bernal stacking. Because of the interlayer interactions, the magnetic energy bands of a bilayer graphene ribbon are different from those of a monolayer ribbon in the Landau-level energies, the energy spacing, the state degeneracy, and the number of the Landau levels. The low-frequency magneto-absorption spectra reveal the characteristics of the electronic properties. The spectra exhibit denser Landau peaks than those of a monolayer ribbon do. Meanwhile, the transition channels of the Landau peaks are also identified. The selection rule is $\Delta n = \pm 1$.

This work was supported by the Taiwan National Science Council (NSC 96-2112-M-165-001-MY3; NSC 95-2112-M-006-0002).

C1.00179 NEGF Transport Simulation on Pd-cluster Functionalized CNTs. CHAO CAO, Quantum Theory Project and Department of Physics, University of Florida, ALEXANDER KEMPER, Quantum Theory Project and Department of Physics, YUAN-HE, Quantum Theory Project, University of Florida, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — We have investigated the conductance response of the Pd-cluster functionalized CNTs to hydrogen environment using DFT+NEGF method. Experiments find that the semiconducting CNTs behave very differently from metallic CNTs, and suggest that the semi-conducting ones are good candidates for hydrogen sensors. By comparing the simulation results for the (5,5) metallic and the (8,0) semiconducting CNTs, we are able to reveal the underlying physics behind this phenomena. This work is supported by the DOE grant number DE-FG02-02ER45995. The authors want to thank NERSC, CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported within this paper.

C1.00180 QUANTUM FLUIDS AND SOLIDS —

C1.00181 Spin-charge separation in a strongly correlated spin-polarized chain. SHIMUL AKHANJEE, YAROSLAV TSERKOVNYAK, UCLA — We combine the first-quantized path-integral formalism and bosonization to develop a phenomenological theory for spin-charge coupled dynamics in one-dimensional ferromagnetic systems with strong interparticle repulsion, at low temperatures. We assume an effective spin-charge separation and retain the standard Luttinger-liquid plasmon branch, which is explicitly coupled to a Heisenberg ferromagnetic spin-wave texture with a quadratic dispersion. The dynamic spin structure severely suppresses the plasmon peak in the single-particle propagator, in both fermionic and bosonic systems. Our analysis provides an effective theory for the new universality class of one-dimensional ferromagnetic systems, capturing both the trapped spin and propagating spin-wave regimes of the long-time behavior.

C1.00182 Implementation of High Temperature Superconducting Leads in research cryostats. YUKO SHIROYANAGI, Ohio State University, GOKUL Gopalakrishnan, DONGKYUN KO, SANGHUN AN, Thomas Gramila, Ohio State University, THOMAS GRAMILA, Ohio State University — High Temperature Superconducting (HTSC) Magnet Leads are available for use in high current applications, which combined with active cryocoolers, they are typically not used in liquid Helium based research cryostats because of the difficulty of implementation. We have successfully implemented a HTSC lead system for Helium based cryostats in which baffles provide thermal coupling to the outgoing Helium gas. The increase in the Helium boiloff rate at full current (110amps) has been measured to be 0.4L/day as compared with the zero current boiloff. An essential element of the design is maintaining a temperature at the warm end of the HTSC leads which is well below the critical temperature. Measurements indicate that this temperature is roughly 65K at 110A. The basic design approach and actual implementation of this novel HTSC lead system, as well as its measurement, are discussed.

C1.00183 QUANTUM INFORMATION, CONCEPTS, AND COMPUTATION I —

C1.00184 PT-Symmetric Quantum Evolution and Logic. TOREY SEMI, MARK COFFEY, Colorado School of Mines — There has been much recent interest in PT-symmetric quantum mechanics (QM) as an alternative formulation of quantum theory. We investigate the potential of this formulation for quantum computation and simulation. PT-symmetric QM replaces the usual postulate that a system’s Hamiltonian must be Hermitian. It argues instead that the Hamiltonian can be symmetric with respect to combined parity and time-reversal and, for certain parametric regions, still produce real eigenvalues and maintain unitary time evolution. Besides being of fundamental interest, this approach allows for a fresh perspective on many QM applications. It is known that for one-qubit PT-symmetric systems the evolution time from an initial state to a final state can be made arbitrarily small. We report on applying PT-symmetric Hamiltonians for two-qubit systems to quantum logic.

C1.00185 Two-particle Interferometry with Filtering Operations. S.-S. B. LEE, H.-S. SIM, Korea Advanced Institute of Science and Technology — We generalize the conventional two-particle interferometer by including filtering operations. We find that after appropriate local filtering operations, the concurrence, a two-particle entanglement measure, can be directly obtained from the visibility of the two-particle interference, even for mixed states. This indicates that entanglement is associated with experimentally feasible properties.

C1.00186 Entanglement of magnetic impurities via electron scattering with asymmetric coupling constants. GUILLEMERO CORDOURIER-MARURI, ROMEO DE COSS, Cinvestav Unidad Mérida, YASSER OMAR, Technical University of Lisbon — We study the entanglement generated by electron scattering between two fixed magnetic impurities, located in a 1-D quantum wire. The impurities were considered distant and only interact through the spin of a scattered electron. We analyzed the asymmetric case produced by the effect of considering different exchange coupling electron-impurity factor for each impurity. We used the quantum waveguide theory approach to find the probability of electron transmission for each spinorial configuration of the system, taking into account the possible changes in the directions of the impurities and electron spins. We find resonance behavior in the evolution of the probability of electron transmission with respect to the impurities separation. We show results for the cases where the average and the difference of the exchange coupling electron-impurity factor are constant. From the probabilities of electron transmission the entanglement is calculated using the von Neumann entropy. We show that the entanglement can be maximized changing the initial conditions of the system, like the impurities separation distance and the ratio of the electron-impurity exchange coupling factor.
C1.00187 Squeezed State Effects on Continuous Variable Quantum Erasing. PETER BONANNO, VIJAY KASISOMAYAJULA, ONOFRIO RUSSO, New Jersey Institute of Technology — Experimental verification of complementarity using quantum erasing for the continuous variable (CV) infinite dimensional Hilbert space has been considered. [1] The complementary pair is that of the canonically conjugate amplitude and phase quadratures of light. The amplitude quadrature is labeled to a squeezed meter signal by quantum nondemolition (QND) [2] entanglement coupling. [3] Knowledge of which eigenstate (WE) can be obtained by measuring this amplitude in the meter state, and can thereafter be ‘lost’ by measuring the quadrature phase of the meter, thus restoring the quadrature phase of the signal beam in a process known as quantum erasure. [4] The coupling, i.e., the labeling of the signal state to the meter state, is implemented with a beam splitter coupled to the squeezed light meter beam. [4] We investigate the effects of using the unitary squeeze operator $S(z) = \exp(2z^2 - z^2)$ where $z = \exp(i\phi)\sqrt{s_{\text{q}}}$. [5] We show that the final state of the meter is a displaced squeezed coherent state $|\alpha\rangle$. [5] The experiment is performed using a squeezed beam as input. The results show that the phase of the meter, thus restoring the quadrature phase of the signal beam in a process known as quantum erasure. [6] The experiment demonstrates the complementarity of amplitude and phase quadratures. 

C1.00188 Hidden variables in quantum mechanics: Generic models, set-theoretic forcing, and the appearance of probability. ROBERT A. VAN WESEP — The hidden-variables (HV) program in quantum mechanics proposes that physical states have properties that are not observable in the ordinary sense and which uniquely determine the outcome of any observation. It is well known that one cannot consistently assign values to all propositions in a Hilbert space of dimension $\geq 3$, but for systems of commuting propositions one always can, so there is some interest in HV in this limited setting. But the same objection has been raised against HV as against the many-worlds view (MW), viz., that it cannot accommodate the notion of probability, specifically the Born rule. We have shown that the Born rule is actually derivable in MW[1]. In the present work we do the same in the HV setting[2]. Specifically, we show that the HV premise implies that the sequence of values assigned by a given HV state to a set of commuting propositions is indistinguishable from a sequence randomly generated according to the Born rule. In fact, the same is true for systems of noncommuting propositions satisfying a natural condition[3]. The sequences demanded by HV are generic in the set-theoretic sense. The fascinating ontology of generic objects in set theory therefore applies to HV states in physics.

C1.00189 Intrinsic Friction Microscopy. DANIEL KNORR, RENE OVERNEY — A novel scanning probe methodology based on lateral force microscopy is presented wherein kinetic friction measurements, obtained as a function of velocity for various temperatures, are used to deduce apparent Arrhenius-type activation energies for surface and subsurface molecular mobilities. Depending on the coupling strength (cooperativity) between molecular mobilities involved the dissipation energy can carry a significant entropic energy contribution, accounting for the majority of the apparent Arrhenius activation energy. The intrinsic friction methodology also provides a means of directly separating enthalpic energy contributions from entropic ones by employing absolute rate theory. As such, the degree of cooperativity in the system is readily apparent. This methodology is illustrated with nanoscale tribological experiments on two systems, (1) monodisperse, atactic polystyrene and (2) self assembling molecular glassy chromophores. In polystyrene, dissipation was found to be a discrete function of loading, where the $\gamma$-relaxation (phenyl group rotation) was recovered for ultra low loads and the $\beta$-relaxation (local backbone translation) for higher loads in the same temperature range, indicating sensitivity to surface and subsurface mobilities. For self assembling glassy chromophores, the degree of intermolecular cooperativity was deduced using the methodology, resulting in an increased understanding of the interactions between self assembling molecules.

C1.00190 HIGH PRESSURE PHYSICS –

C1.00191 Influence of Shockwave Profile on Ejection of Micron-Scale Material From Shocked Tin Surfaces. MICHAEL ZELLNER, JIM HAMMERBERG, ROBERT HIXSON, RUSSEL OLSON, PAULO RIGG, Los Alamos National Lab, GERALD STEVENS, WILLIAM TURLY, National Security Technologies, WILLIAM BUTTLER, Los Alamos National Lab — This effort investigates the relationship between shock-pulse shape and the amount of micron-scale fragments ejected (ejecta) upon shock release at the metal/vacuum interface of shocked Sn targets. Two shock-pulse shapes are considered: supported shock created by impacting a Sn target with a sabot that was accelerated using a powder gun; and an unsupported or triangular-shaped Taylor shockwave, created by detonation of high explosive that was press-fit to the front-side of the Sn target. Ejecta production at the back-side or free-side of the Sn coupons were characterized through use of piezoelectric pins, Asay foil, optical shadowgraphy, and X-ray attenuation.

C1.00192 Pressure induced valence changes in YbTe studied by resonant inelastic x-ray emission (RXES)1. RAVHI KUMAR, ANDREW CORNELIUS, HiPSEC, Dep.Physics and Astronomy, UNLV, Las Vegas, NV 89154, YUMING XIAO, PAUL CHOW, HPCAT and Carnegie Institution of Washington, Advanced Photon Source, Argonne, IL, MALCOLM NICOL, HiPSEC, Dep.physics and Astronomy, UNLV, Las Vegas, NV 89154 — We have performed high resolution x-ray absorption (XAS) and resonant inelastic x-ray emission (RXES) experiments to probe the pressure dependence of Yb valence in YbTe as high as 20 GPa. XAS spectra were collected in the partial fluorescence yield (PFY) mode at the Yb L3 edge. The RXES spectra were recorded by fixing the incident energy and collecting the transferred energy as a function of pressure in 2eV steps. The results show a continuous valence change of Yb towards 3+ from the mixed valent state, similar to other mixed valent Yb compounds under pressure [1, 2]. The experimental details with the PFY and RXES results will be presented. 1. C. Dallera, M. Grioni, A. Shukla, G. Vanko, L. Bravicoh, A. Shukla and M. Grioni, Phys. Rev. B., 68, 245114 (2003)

C1.00193 Sugar pucker in nucleosides as a function of pressure. SCOTT LEE, University of Toledo — Infrared and Raman experiments of adenosine (rA), deoxyadenosine (dA), cytidine (rC) and deoxycytidine (dC) have been performed at room temperature as a function of pressure. Phase transitions are observed to occur near 2 and 4 GPa in rA and dA and near 4 GPa in rC and dC. Based on theoretical calculations of the vibrational frequencies, these transitions appear to be due to changes in the sugar moiety. The most likely explanation is that the sugar pucker changes at these pressures. These observations are relevant to our understanding of the A-to-B transition observed in DNA.

1HiPSEC is supported by DOE, NNSA under co-operative agreement DE-FC08-01NV14049.
C1.00194 First-order polymorphic phase transition in supercooled liquid Silicon. P. GANESH, Carnegie Institution of Washington, MIKE WIDOM, Carnegie Mellon University — We perform first-principles molecular dynamics simulation of liquid and supercooled liquid Silicon. Looking at the volume dependence of the pressure at different supercooled liquid temperatures, we find a van der Waals loop, indicating a possible liquid-liquid first-order phase transition. It appears that the transition can be seen only at pressures of about a few GPa. We analyze our data using the zero-th moment of the tetrahedral order parameter, \( q_i = 1 - \frac{1}{3} \sum_{j<k} \cos[\theta_{ijk} + \frac{1}{2} \pi^2/i(1)] \), where \( \theta_{ijk} \) is the angle formed among neighbors ‘\( j \)’ and ‘\( k \)’ and the central atom ‘\( i \).’ For a perfect tetrahedral arrangement (\( \cos[\theta_{ijk} + \frac{1}{2} \pi^2/i(1)] \)) the value of the order-parameter is ‘1’ and for an uncorrelated system its distribution is peaked at ‘0’. We find that the low temperature liquid has a more tetrahedral open network than the high temperature one, indicating that the transition is between a high-density and a low-density liquid. The electronic density of states along an isocore indicates a sharp drop in metallicity across the transition temperature, which we believe lies around \( T = 1100K \). [1] M. Scott Shell and Pablo G. Debenedetti and Athanassios Z. Panagiotopoulos, Physical Review E 66, 011201, (2002)

C1.00195 Formation of nano-domains during the ZB-B1 high-pressure transition in bulk ZnSe , R.E. TALLMAN, B.A. WEINSTEIN, P. ZHANG, Physics Dept., SUNY at Buffalo, V. IOTA, H. RHEE, Lawrence Livermore National Laboratory, M.A. MARCUS, Lawrence Berkeley Laboratory — Raman scattering and x-ray absorption spectroscopy (XAS) are applied to explore the early-stage nucleation of the zincblende-rocksalt high-pressure transition in ZnSe. The Raman spectra (300K) of both natural ZnSe and high-quality vapor-grown ZnSe exhibit extreme broadening in the region of the TO(\( \Gamma \)) phonon for pressures \( \sim 2.5 \) GPa below the onset of the opaque high-pressure phase. At the same time sharp features persist in the spectra, e.g., due to the resonantly enhanced LO(\( \Gamma \)) peak and the 2TA(\( X \)) and 2TA(\( L \)) critical points. These results indicate that the high-pressure rocksalt phase in ZnSe tends to form in nanoscale domains due to a high density of nucleation sites. In order to explore the nucleation process further, XAS measurements are carried out under applied pressure on a ZnSe film containing \( \sim 10^{21} \) cm\(^{-3} \) As-impurities as an easily identifiable source of nucleation sites. Comparisons of the XAS results at 1 atm. and 6.5 GPa support the early onset of disorder consistent with nano-domain formation and the Raman findings.

C1.00196 A first-principles investigation of ionic vacancies and diffusion in high-pressure silica polymorphs, ASHOK VERMA, BIJAYA KARKI, Department of Computer Science, Louisiana State University, Baton Rouge, Louisiana 70803, USA — We have performed the density functional theory based simulations within the local density and pseudopotential approximations to investigate the effects of pressure and structural changes on the formation and migration energies of the ionic vacancies in crystalline silica. The simulations use supercells of 72 atoms for \( \alpha \)-quartz, stishovite and \( \text{CaCl}_2 \)-type and 96 atoms for \( \alpha \)-\( \text{Fe}_2 \text{O}_3 \) and pyrite type silica. The simulations are performed up to 250 GPa pressure. The atomic positions are fully optimized. Our results show a discontinuous change in Schottky formation enthalpy at phase transitions which involve cation coordination number change. In fact increase in cation coordination number leads in reduction of Schottky formation enthalpy. For example, at 0 GPa pressure Schottky formation enthalpies of 4-fold (\( \alpha \)-quartz), 6-fold (stishovite) and 6(=2)-fold (pyrite) coordinated silica are 16.12 eV, 11.02 eV and 7.73 eV respectively. Calculations of migration enthalpies, activation enthalpies and activation volumes all are also carried out up to 250 GPa pressure.

C1.00197 GENERAL —

C1.00198 Two Theories Are Better Than One , ROBERT JONES, Emporia State University — All knowledge is of an approximate character (B. Russell, Human Knowledge, 1948, pg 497 and 507). Our formalisms abstract, idealize, and simplify (R. L. Epstein, Propositional Logics, 2001, Ch XI and E. Bender, An Intro. to Math. Modeling, 1978, pg v and 2). Each formalism is an idealization, often times approximating in its own DIFFERENT ways, each offering somewhat different coverage of the domain. Having MULTIPLE overlapping theories of a knowledge domain is then better than having just one theory (R. Jones, APS general meeting, April 2004). Theories are not unique (T. M. Mitchell, Machine Learning, 1997, pg 65-66 and Cooper, Machine Learning, vol. 9, 1992, pg 319). In the future every field will possess multiple theories of its domain and scientific work and engineering will be performed based on the ensemble predictions of ALL of these. In some cases the theories may be quite divergent, differing greatly one from the other. This idea can be considered an extension of Bohr’s notion of complementarity, "...different experimental arrangements...described by different physical concepts...together and only together exhaust the definable information we can obtain about the object." (H. J. Folse, The Philosophy of Niels Bohr, 1985, pg 238)

C1.00199 What’s in a Name?FRAMING:Martin-Bradshaw DYSfunctionality = Siegel “Buzzwordism,Bandwagonism&$Sloganeering For: Fun, Profit,Survival,Ego”: From SOC to FLT Proof to High-Tc to Spintronics to Giant-Magnetoresistance: Ethics?? SHMETHICS!!!

Rampant Sociology , EDWARD SIEGEL — Buzzwordism,Bandwagonism,Sloganeering for Fun,Profit,Survival,Ego: From SOC to FLT Proof to High-Tc to Spintronics to Giant-Magnetoresistance: Ethics?? SHMETHICS!!!

C1.00200 GENERAL THEORY INCLUDING COMPUTATIONAL METHODS: MANY BODY AND STRONGLY CORRELATED SYSTEMS —

C1.00201 A nonlinear quantum master equation symmetric with respect to particles and holes , C.F. HUANG, CMS/ITRI, K.-N. HUANG, Department of Physics, NTU — A nonlinear master equation symmetric with respect to particles and holes has been introduced for systems composed of non-interacting identical fermions. [1,2] It can be reduced to semiclassical irreversible equation in the incoherent limit, and can be generalized to model interacting and/or open quantum systems. [2,3] To prove the validity of Pauli’s exclusion principle, we note that such a principle holds true if and only if the density matrix for holes is a positive one. Suitable mathematical structures have been constructed to complete the proof when there exists an upper bound for the transition rate. Extensions based on BCS-type symmetry are taken into account to incorporate both particle-particle and particle-hole pairings. References: [1] K. Burke, R. Car, and R. Gebauer, Phys. Rev. Lett. 94, 146803 (2005) [2] C. F. Huang and K. –N. Huang, quant-ph/0604054. [3] R. Alickij and K. Lendi, “Quantum Dynamical Semigroups and Applications” (Springer, Berlin Heidelberg 2007)
C1.00202 A new Variational Approach to the Hydrogen Atom, I. DJURIC, F.A. CORVINO, Stevens Institute of Technology, V. FESSATIDIS, Fordham University, J.D. MANCINI, Kingsborough College of CUNY — Over a decade ago, a systematic scheme for improving the variational wave functions and corresponding energy levels for quantum systems was developed. By expanding the wave function around a variational parameter value(s), a family of independent functions may be systematically generated. The eigenstates are then obtained by diagonalizing the Hamiltonian basis and optimized with respect to variational parameter(s). In this work we wish to apply this scheme to the well studied and understood ground state of the hydrogen atom. For a trial (starting vector) state we make two choices: \( e^{-\alpha r} \) and \( e^{-\beta r} \) where \( \alpha \) and \( \beta \) are variational parameters. Our two (variational) basis are then constructed by taking derivatives with respect to these parameters. We then choose a linear combination of the two states \( e^{-\alpha r} \) and \( e^{-\beta r} \) as our initial state and minimize with respect to both parameters. This leads to questions of the optimal number of each derivative \( \frac{\partial \psi}{\partial \alpha} \), \( \frac{\partial \psi}{\partial \beta} \), which will yield the lowest ground state energy for a given basis size \( N \) (\( \mu + q = N \)).

C1.00203 Variational Bond States of Screened Potentials, J.D. MANCINI, Kingsborough College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University, W.J. MASSANO, SUNY Maritime — A number of years ago, a calculational scheme was introduced by Stubbins (Phys. Rev. A48, 220 (1993)) to compute the energies of both the Hulthén and Yukawa potentials. The method introduces a particular ansatz for solving the Schrödinger equation with screened Coulomb type potentials. In this work we wish to review the method of Stubbins and to show that it is, in fact, equivalent and a subset of a more systematic (and hence more useful) variational scheme (Zhou et al. Phys. Rev. A51, 3337 (1995)). This variational approach involves the construction of a basis by taking derivatives of the variational parameters of the system. The eigenvalues of the Hamiltonian matrix are then minimized with respect to these parameters yielding a “best guess” upper bound on the energies.

C1.00204 Translational Invariance in Parameter Space: An Alternate Variational Coupled Cluster Method, V. FESSATIDIS, Fordham University, J.D. MANCINI, Kingsborough College of CUNY, S.P. BOWEN, Chicago State University, R.K. MURAWSKI, Drew University — Over the past few decades the Coupled Cluster Method (CCM) has proven to be a useful tool for both chemists and physicists in the calculation of ground state energies. The CCM scheme is also a viable method in calculating the correlation energies of a number of diverse quantum systems such as atoms, molecules, electron gases as well as for magnetic lattice systems. In this work a new many-body calculational scheme is developed by merging the CCM scheme with a relatively new variational ansatz wherein a basis is constructed by taking derivatives with respect to the variational parameters of the system. A novel translational operator is then introduced leading to a generalization of Bloch’s Theorem in parameter space.

C1.00205 Microsolvation Effects on the Excited-State Dynamics of Protonated Tryptophan, MATTEO GUGLIELMI, SEBASTIEN MERCIER, OLEG BOYarkin, ANTHI KAMARIOTIS, IVANO TAVERNELLI, MICHELE CASCELLA, URSULA ROETH- LISBERGER, THOMAS RIZZO, LCPC COLLABORATION — To better understand the complex photophysics of the amino acid tryptophan, which is widely used as a probe of protein structure and dynamics, we have measured electronic spectra of protonated, gas-phase tryptophan solvated with a controlled number of water molecules and cooled to ~10 K. We observe that, even at this temperature, the bare molecule exhibits a broad electronic spectrum, implying ultrafast, nonradiative decay of the excited state. Surprisingly, the addition of two water molecules sufficiently lengthens the excited-state lifetime that we obtain a fully vibrationally resolved electronic spectrum. Quantum chemical calculations at the Rl-CC2/aug-cc-pvdz level, together with TDFT/pw based first-principles MD simulations of the excited-state dynamics, clearly demonstrate how interactions with water destabilize the photodissociative states and increase the excited-state lifetime.

C1.00206 The One-Hole, One-Dimensional Hubbard Model at \( U = \infty \), WILLIAM HODGE, NATALIE HOLZWARTH, WILLIAM KERR, Wake Forest University — The Hubbard Hamiltonian is the simplest model that describes interacting electrons on a lattice. In this work, we use the properties of stochastic matrices to examine the ground state with an even number of lattice sites and one electron less than half-filling. We show that there exists a highly symmetric state with energy \(-2\) (in units where \( t = 1 \)) at all \( U \). At \( U = \infty \) this state becomes the lowest energy state, consistent with the established lower energy bound.\footnote{S. A. Trugman, Phys. Rev. B 42, 6612 (1990)} Using this result, several properties of the strongly coupled ground state are derived, including the chemical potential and momentum distribution. This method may be applicable to other models as well. Disagreements between our results and previous work are examined.

C1.00207 Direct extension to \( n \)-leg models in the density-matrix renormalization group method: An approach on the ground state of two-dimensional triangular Hubbard model, SUSUMU YAMADA, MASAIKO ÔKUMURA, MASAIKO MACHIDA, CCSE, Japan Atomic Energy Agency — In order to examine the ground state of two-dimensional triangular Hubbard model, we directly extend the density-matrix renormalization group (DMRG) method to \( n \)-leg lattice model. The leg extension requires not only an enormous memory space but also a huge CPU cost. Therefore, we propose an efficient and scalable parallel algorithm of the direct DMRG method and actually perform parallel numerical simulations of triangular 4- to 6-leg Hubbard models using 128 to 512 CPUs on SGI Altix 3700Bx2 in JAEA. In this presentation, we will briefly introduce the parallelization strategy, the implementation way, and show its performance including its scalability and accuracy. Furthermore, we reveal peculiar particle density distributions on \( n \)-leg triangular Hubbard models. These results are compared with the future experiments on atomic Fermi gases loaded on triangular optical lattices.\footnote{CREST (JST)}

C1.00208 s-Wave Superconductivity Phase Diagram in the Inhomogeneous Two-Dimensional Attractive Hubbard Model, KARAN ARYANPOUR, Department of Physics, SUNY at Buffalo, THEREZA PAIVA, Universidade Federal do Rio de Janeiro, Brazil, WARREN E. PICKETT, RICHARD T. SCALLETAR, Department of Physics, University of California, Davis — We study s-wave superconductivity in the 2-D square lattice attractive Hubbard Hamiltonian for inhomogeneous patterns of interacting sites. Using the Bogoliubov-de Gennes ( BdG) mean field approximation, we obtain the phase diagram for inhomogeneous patterns with on-site electron interaction \( U \) taking on two values, 0 and \(-U/(1-f)\) (\( f \) the non-interacting sites concentration) as a function of electron density per site \( n \) as \( f \) varies. Inhomogeneity can result in a larger average pairing amplitude at \( T = 0 \) and also a higher superconducting \( T_c \), relative to a uniform system. Superconductivity can also vanish due to charge ordered phase formation. \( T_c \) enhancement due to inhomogeneity is robust as long as \( n < 2(1-f) \) regardless of the pattern. Also, for certain inhomogeneous patterns, when \( n = 2(1-f) \), raising temperature works against the stability of existing charge ordered phases for large \( f \) and as a result, enhances \( T_c \).

\footnote{We acknowledge NSF Grants DMR-0421810, DMR-0426826, US ONR, CNPq-Brazil and FAPERJ-Brazil.}
C1.00209 Simple dynamic exchange-correlation kernel of the uniform electron gas\(^1\), LUCIAN constatin, J.M. pitarke, Tulane University — We propose a simple dynamic exchange-correlation kernel of the uniform electron gas. We model the reduction of the electron-electron interaction due to short-range exchange-correlation effects by introducing a frequency-dependent error-function effective interaction. By imposing the fulfillment of the compresibility and the third-frequency-moment sum rules, as well as the correct asymptotic behavior at large wave vectors, we find an accurate and simple dynamic exchange-correlation kernel that accurately reproduces the wave-vector analysis and the imaginary-frequency analysis of the correlation energy of the uniform electron gas.

\(^1\) We acknowledge partial support by the University of the Basque Country, the Basque Unibertsitate eta Ikerketa Saila, the Spanish Ministerio de Educacion y Ciencia, and the EC 6th framework Network of Excellence NANOQUANTA-Grant No. NMP4-CT-2004-500198.

C1.00210 Critical parameters for the disorder-induced metal-insulator transition in FCC and BCC lattices, Andrzej eilmes, Department of Computational Methods in Chemistry, Jagiellonian University, Krakow, Poland, Andrea M. Fischer, Rudolf A. Roemer, Department of Physics and Centre for Scientific Computing, University of Warwick, UK — We use a transfer matrix method to study the disorder-induced metal-insulator transition for. We take isotropic nearest- neighbour hopping and an onsite potential with uniformly distributed disorder. Following previous work done on the simple cubic lattice, we perform numerical calculations for the face centred cubic (FCC) and body centred cubic (BCC) lattices, which are more common in nature. We obtain the localisation length from calculated Lyapunov exponents for different system sizes. This data is analysed using finite size scaling to find the critical parameters. We create an energy-disorder phase diagram for both lattice types, noting that it is symmetric about the band centre for the BCC lattice, but not for the FCC lattice. We find a critical exponent of approximately 1.5-1.6 for both lattice types for transitions occurring either at fixed energy or at fixed disorder, agreeing with results previously obtained for other systems belonging to the same orthogonal universality class. We notice an increase in critical disorder with the number of nearest neighbours, which agrees with intuition.

C1.00211 The Gutzwiller Ansatz: A new Approach, J.D. Mancini, Kingsborough College of Cuny, V. Fessatidis, Fordham University, I. Djuric, Stevens Institute of Technology, S.P. Bowen, Chicago State University — The search for calculational methods for dealing with strongly correlated electron systems ranging from high Tc superconducting compounds and other transition metal oxide materials to f-electron bearing elements is a long and continuous one. There are a number of well documented failures of such schemes as the local density approximation and the generalized gradient approach. Although these methods partially address the issues related to the strongly correlated electrons, a comprehensive theory is still lacking. The choice of including electrons correlations using the Gutzwiller variational wave function has proved over the years to be a useful one in the interpolation between the strong electron correlation (large U) and weak electron correlation (small U) limits. In this work a novel variational ansatz is applied to strongly correlated systems by using the Gutzwiller wave function as our initial vector, and then systematically constructing a basis by taking derivatives with respect to the variational parameters of the system. The eigenvalues of the Hamiltonian matrix with this basis are then minimized to yield a variational upper bound on the ground state energy.

C1.00212 Solution of the Electron Fluid Dynamical Equations, Mostafa Hemmati, Arkansas Tech University — To describe the breakdown waves, we use a one-dimensional, steady-state, three-fluid, hydro-dynamical model with a shock front. We assume that the electron gas partial pressure is much larger than the partial pressures of the other species and therefore provides the driving force for the propagation of the wave. The wave is composed of two distinct regions: a thin dynamical transition layer followed by a relatively thicker thermal layer. In the transition region, the electrons slow down to speeds comparable to those of heavy particles as the electric field fails to zero. In the thermal layer, the high temperature electron gas will cool, resulting in more ionization. The set of equations used to investigate these waves consists of the equation of conservation of mass, momentum, and energy coupled with Poisson’s equation, and is known as the electron fluid dynamical (EFD) equations. We have replaced the assumption of ionization rate being a function of temperature only, by a computation based on the free trajectory theory by Fowler; in which the ionization rate changes from accelerationnal ionization at the front of the wave to directed velocity ionization in the intermediate stages of the wave to thermal ionization at the end of the wave. Using Fowler’s equation to calculate the ionization rate, we have been able to integrate the EFD equations through both, the transition and thermal layers of the wave. The results conform to the expected conditions at the end of both layers. Wave profile for the electric field, ionization rate, and electron velocity, temperature, and number density will be presented.

C1.00213 INSTRUMENTATION AND MEASUREMENTS —

C1.00214 Branching Transport Model of NaI (Tl) Scintillator\(^1\), Boian Alexandrarov, Lanl and University of New Mexico, Kiril Ianakiev, Lanl, Peter Littlewood, Cavendish Laboratory, UK — The time dependence of NaI(Tl) fluorescence was measured long time ago with the delayed coincidences method and two decay time components were observed. Because 95% of the total light yield is collected within the first 800 ns, the influence of the second component has been neglected. We claim that there are two dominant time components with strong temperature redistribution. We experimentally measured the time dependence of the NaI(Tl) light-emission pulses and found that the amplitude ratio of these two components shows Arrhenius temperature dependence. We found that the slow component occupies up to 40% of total light at -20\(^\circ\)C temperature. We analyze the time shape of the light pulse to directed velocity ionization and rotation K\(^\theta\).

\(^1\) Work supported by NSF through career DMR-0547887, the Nebraska Research Initiative, and the NSF MRSEC Program DMR-0213808.

C1.00215 Optimization of MOKE Setups: Analyzing Experimental Assemblies Using Jones Matrix Formalism\(^1\), Srinivas Polisetty, jeremy scheffler, Sarbeswar sahoo, Christian binek, University of Nebraska-Lincoln — We report on the optimization of Magneto Optical Kerr setups. Photoelastic modulation and phase sensitive detector methodology have been used to measure the first and second harmonics of the reflected light intensity related to the magnetization-dependent off-diagonal reflection coefficients \(r_{pa}/sp\) of the sample’s dielectric tensor. The latter elements determine the Kerr ellipticity \(\varepsilon_K\) and rotation \(\theta_K\). Jones matrix formalism has been used to analyze a large variety of arrangements of the optical elements involved in setups for longitudinal Kerr measurements with incoming s-polarized light. Relative analyzer and polarizer orientations have been varied with respect to each other and with respect to the retardation axis of the modulator. Different configurations have been analyzed and experimentally studied by measuring magnetic Kerr-hysteresis loops on a Co/CoO bilayer sample. We find that one configuration stands out by doubling the first as well as second harmonic intensities and, hence, the signal to noise ratio. Inefficient setups show first and second harmonic signals involving non-magnetic background contributions of \(r_p\) and \(r_s\).

\(^1\) Work supported by NSF through career DMR-0547887, the Nebraska Research Initiative, and the NSF MRSEC Program DMR-0213808.
C1.00216 Electromagnetic modulation of the ultrasonic signal for nondestructive detection of small defects and ferromagnetic inclusions in thin wall structures, PETER FINKEL, Drexel University — We report on new nondestructive evaluation technique based on electromagnetic modulation of ultrasonic signal for detection of the small crack, flaws and inclusions in thin-walled parts. The electromagnetically induced high density current pulse produces stresses which alter the ultrasonic waves scanning the part with the defect and modulate ultrasonic signal. The excited electromagnetic field can produces crack-opening due to Lorentz forces that increase the ultrasonic reflection. The Joule heating associated with the high density current, and consequent thermal stresses may cause both crack-closure, as well as crack-opening, depending on various factors. Experimental data is presented here for the case of a small crack near holes in thin-walled structures. The measurements were taken at 2-10 MHz with a Lamb wave wedge transducer. It is shown that electromagnetic transient modulation of the ultrasonic echo pulse tone-burst suggest that this method could be used to enhance detection of small cracks and ferromagnetic inclusions in thin walled metallic structures.

C1.00217 Detection of nerve agents and biological molecules using embedded piezoresistive microcantilever sensors, TIMOTHY PORTER, TIM VAIL, AMANDA WOOLEY, Northern Arizona University — Embedded piezoresistive microcantilever (EPM) sensors have been used in the detection of a variety of analyte species. EPM sensors utilize a tiny piezoresistive microcantilever partially embedded into a sensing material to produce a sensing element that is compact, simple, resistant to movement and shock, and suitable for remote sensing applications. In the current project, we have used sensing materials comprised of an immobilizing polymer functionalized with either target enzymes or antibodies to detect two biological agents, bacillus globigi (BG) and Dilsopropyl fluorophosphate (DFP). DFP is an organophosphate used as a simulant for organophosphate nerve agents, while BG is a large bacterial spore used as a simulant for other bacterial spores such as bacillus anthracis. Sensing results are presented for both types of EPM sensors.

C1.00218 Micro-Oscillators for Ultra-Sensitive Force Detectors, WEI LU, JOHN MARKERT, Physics Department, University of Texas at Austin — Recently, we have improved the microfabrication process for ultra-sensitive double-torsional mechanical micro-oscillators. Starting with silicon-on-insulator wafers (with 300 nm Si surface layers), we grow a protective layer of oxide, then pattern 2-mm × 0.5-mm “windows” that result in a thin Si film after two-sided wet chemical etching. Patterning these film windows with electron-beam lithography then provides the final micro-oscillator structures. Our designs include multimode structures, particularly double-torsional modes; we have achieved excellent geometric symmetry and small sizes (~30 μm laterally and 300 nm thick). These oscillators have excellent force sensitivity, yet provide stronger mechanical structures than typical ultrafloppy cantilevers designs. For example, an antisymmetric double-cantilever mode provides a minimum detectable force of 1.6 × 10⁻¹⁶ N/√Hz at 3He temperatures. A double torsional mode typically provides enhanced sensitivity, so minimum detectable forces on the order of 10⁻¹⁹–10⁻²⁰ N/√Hz are now targeted.

1This work was supported by the NSF under Grant DMR-0605828.

C1.00219 Surface Plasmon Based Spectrometer, ANDREW WIG, Benedictine University, ALI PASSIAN, PHILIP BOUDREAU, TOM FERRELL, University of Tennessee — A spectrometer that uses surface plasmon excitation in thin metal films to separate light into its component wavelengths is described. The use of surface plasmons as a dispersive medium sets this spectrometer apart from prism, gratings, and interference based variants and allows for the miniaturization of this device. Theoretical and experimental results are presented for two different operation models. In the first case surface plasmon tunneling in the near field is used to provide transmission spectra of different broad band-pass, glass filters across the visible wavelength range with high stray-light rejection at low resolution as well as absorption spectra of chlorophyll extracted from a spinach leaf. The second model looks at the far field components of surface plasmon scattering.

1This work was supported by the Defense Advanced Research Projects Agency (DARPA)
2Oak Ridge National Laboratory

C1.00220 Atomic Force Microscopy Simulation in Aqueous Environment by RISM Theory, MASANORI HARADA, MASARU TSUKADA, Waseda University — Many theoretical simulations of atomic force microscopy (AFM) have been performed so far to clarify the underlying physics in experimental AFM images which were difficult to understand intuitively. Most of the simulations use the models consisting of only tip and sample atoms and successfully reproduce experimental AFM images obtained in vacuo. However, those models are not suitable to simulate the AFM experiments performed in liquid or gaseous environments. Reference Interaction Site Model (RISM) is used in our simulation to incorporate liquid effect. This method is based on statistical mechanics and has the advantage of low computational cost over all-atom molecular dynamical simulations. To investigate the efficiency of the method, we simulated the force-distance curves and 2D force maps in constant height mode for two different operation models. In the first model the flight path is a factor of two longer than used in previous TOF-PAES systems. The longer flight path is expected to result in a fractional energy width: δE/ E = 5 × 10⁻¹⁸ N/√Hz at 3He temperatures. A double torsional mode typically provides enhanced sensitivity, so minimum detectable forces on the order of 10⁻¹⁹–10⁻²⁰ N/√Hz are now targeted. 1

1This work was supported by the Defense Advanced Research Projects Agency (DARPA)
2Oak Ridge National Laboratory

C1.00221 Two Meter Flight Path - Time of Flight Positron Annihilation Induced Auger Electron Spectrometer, S. MUKHERJEE, K. SHASTRY, W. ADDOX, A. H. WEISS, U. Texas at Arlington — Details of the design and construction of a new time of flight positron annihilation induced Auger electron (TOF-PAES) spectrometer are presented. The new spectrometer will be equipped with a 2 meter long “TOF” tube that can be biased at a potential different from that of the sample in order to increase or decrease the kinetic energy of the electrons traveling through the tube. The time of flight will be determined from timing signals obtained from the detection of the annihilation gamma (signaling the start of the flight) and detection of the annihilation induced Auger electron at the end of the 2 meter flight path (signaling the end of the flight). The 2 meter long flight path is a factor of two longer than used in previous TOF-PAES systems. The longer flight path can be expected to result in a fractional energy width: δE/ E that is 1/2 as large as the current UTA lab based TOF-PAES spectrometer.

1Y-1100 Welch Foundation

C1.00222 Theoretical simulation of nc-AFM images of mica surface in water, KATSUNORI TAGAMI, MASARU TSUKADA, Waseda University — Based on molecular dynamics simulations, the non-contact atomic force microscopy (nc-AFM) images are simulated of mica surface in water. The tip is modeled by the carbon nanotube apex and the temperature is assumed to be 300 K. The interatomic interactions used in the calculations are listed in CHARMM22 and CLAY force field models. The force curves show oscillatory behaviours near the surface and their amplitudes are found to significantly depend on the scanning points, which produces highly resolved images of the surface structure. In the talk we will make a presentation on the relationship between the normal force and water density profile.
C1.00223 Micromechanical force detectors for measuring magnetization at high magnetic fields and the magnetic response of Ba3Cr2O8. K. NINIOS, H.B. CHAN, UF, Y. J. JO, L. BALICAS, FSU, A. ACZEL, McMaster University, G. M. LUKE, FSU — We report magnetization measurements of Ba3Cr2O8 using micromechanical Faraday balance magnetometers. The magnetometers consist of a movable polysilicon plate (500 by 500 micrometers) supported by four springs 2.75 micrometers above a fixed electrode. When small samples of the magnetic material are placed at the center of the movable plate, the natural gradient of the field creates a force on the sample that changes the capacitance between the plate and electrode, while the response to magnetic torque is minimized. The absolute magnetization of the sample can be determined provided that the magnetic field gradient is known. The device is used to measure the magnetization of a small sample of Ba3Cr2O8 with mass of 1 microgram. At high fields, our measurements reveal an asymmetric dome like structure in the temperature-magnetic field phase diagram, possibly related to the Bose-Einstein condensation of spin triplet degrees of freedom.

C1.00224 Characterization and Modeling of Off-Specular Neutron Scattering for Analysis of Two Dimensional Ordered Structures. CHRISTOPHER J. METTING, ROBERT M. BRIBER, University of Maryland, JULIE A. BORCHERS, BRIAN MARANVILLE, PAUL KIENZLE, CHUCK F. MAJKRZAK, JOSEPH A. DURA, NCNR — Work is currently being done to expand further neutron reflectometry to the off-specular regime for the characterization of thin films with two-dimensional, ordered in-plane structures. The combination of this two-dimensional, in-plane information with the depth-profile that is routinely obtained from reflectivity data can produce a complete, 3-D description of both the structure and magnetic characteristics of these films. The University of Maryland along with the NIST Center for Neutron Research (NCNR) are developing software which can easily be integrated into existing neutron modeling package such as ReflpaK, and will expand the accessibility of off-specular neutron reflectometry to the general scientific community. In this presentation, we show data obtained using a position sensitive detector on the AND/R instrument at the NCNR facility for a range of model systems. Preliminary analysis has been completed on several sample sets with wire and diffraction grating geometries. In addition, patterned gold samples are being lithographically produced in order to test models for a variety of standard feature structures and patterns.

C1.00225 Upgraded varied-line-space PCM beamline at CAMD. PINCHENG ZHOU, EZIZI MORIKAWA, CAMD, Louisiana State University, 6980 Jefferson Hwy, Baton Rouge, LA 70806 — CAMD is a synchrotron research center at the Louisiana State University. Recently, the center’s aging plane-grating vuv soft x-ray monochromator beamline was upgraded to a varied-line-space plane-grating monochromator beamline. Preliminary experiments show performance improvements in the resolving power from 1000 to 5000 and the throughput from 109 to 1011 photons/sec.100 mA. A polarization aperture providing right and left circular polarized photon beams from the bending magnet radiation is scheduled to be installed in the front-end section of this beamline that will provide the opportunity to perform X-ray Magnetic Circular Dichroism(XMCD) spectrum experiments spectroscopy in the future.

C1.00226 Free-electron laser-based pulsed electron paramagnetic resonance, SUSUMU TAKAHASHI, MARK S. SHERWIN, GERALD RAMIAN, University of California Santa Barbara, LOUIS-CLAUDE BRUNEL, JOHAN VAN TOL, National High Magnetic Field Laboratory — High-power pulsed electron paramagnetic resonance (EPR) is extremely useful to study the ultrafast dynamics of spins. At present, most high-power pulsed EPR spectrometers operate near the X-band frequency of 9.5 GHz with kW-level power. A trend in the evolution of next generation pulsed EPR is for higher magnetic field and frequency, both for finer spectral and time resolution and because motional averaging becomes negligible. Since the linewidth of resonances studied by pulsed EPR tends to be extremely narrow, the source radiation also has to be stable and have narrow bandwidth. High-power pulsed EPR, using few-ns pulses to rapidly manipulate spins for spin-echo and related experiments, has been demonstrated at 98 GHz using kW-power Klystron-based sources. A bottleneck for higher frequency pulsed EPR spectroscopy is a lack of sources with high power and narrow bandwidth. The University of California Santa Barbara (UCSB) free-electron lasers (FEL) are potential sources for high-power pulsed EPR because they generate kW of power tunable from 120 GHz to 4.7 THz. We present the current status of the UCSB FEL-based 240 GHz pulsed EPR spectrometer.

C1.00227 Directed Self-assembly of Nanostructures to Develop AFM-Based Biomaterial-to-Electronic Interface, MEHDI YAZDANPANAH, MAHDI HOSSEINI, SANTOSH PABBA, SCOTT BERRY, VLADIMIR DOBRKOTOV, ABDELLILAH SAFIR, ROBERT KEYNTON, ROBERT COHN, University of Louisville, ELECTROOPTICS RESEARCH INSTITUTE AND NANOTECHNOLOGY CENTER TEAM — Very flexible and rugged Ag2xGa nanoneedles of constant diameter (sub 100 nm diameter, 7-70 microns long) can be securely grown onto AFM tips at room temperature. These nanoneedles are electrically conductive and have stiffness well matched to viscoelastic properties of complex fluids and biological materials. This talk specifically presents the abilities of the needles to (1) make precise AFM measurements of surface tension, contact angle, evaporation rate, and shear viscosity of polymeric liquids, (2) measure complex viscoelastic properties of cell membranes and organelles of blood and endothelial cells, (3) capture and be surrounded by single live endothelial cells within a few seconds, (4) polymerize and detect the growth of protein nanofibers on the end of the nanoneedles and (5) functionalize the end of the needles with protein nanofibers and use them for imaging the cell receptors.

C1.00228 Force measurement with a scanning tunneling microscope, KAI-FELIX BRAUN1, SAW-WAI HLA, Ohio University — We present a method to measure the interaction force between single atoms with a scanning tunneling microscope [1]. During experiments for atomic manipulation with a scanning tunneling microscope the tip height curve is recorded. It is shown here that the amplitude of the manipulation curve is a measure for the interaction force between the microscopes tip and a single atom adsorbed on a surface. A simple formula is derived and tested. Extensions of this scheme to different surfaces shall be discussed. [1] K.-F. Braun and S.W. Hla, Physical Review B 75 (2007), 033406.

C1.00229 ESR-MRI Using Low-Temperature Magnetic Resonance Force Microscopy, SHIGENORI TSUIJI, TATSUYA FUJIMOTO, YOHSUKE YOSHINARI, JEOL Ltd., CREST, KOHSUKE INOMATA, Kyoto Univ., CREST — The low-temperature operation of Magnetic Resonance Force Microscopy (MRFM) leads to a significantly better signal-to-noise ratio (SNR) than at room temperature, because of an increase of the spin magnetization and a reduction of the thermo-mechanical noise of the cantilever. We have built a low-temperature equipment, which is capable of operating in vacuum at liquid helium temperature. Our setup employed the sample-on-cantilever design at present. A magnetic needle with 100Å in diameter was placed on a stage to generate magnetic field gradient 11.3 G/µm at the magnetic field 7 T. The 3D closed-loop stage based on slip-stick principle allows a 200 x 200 x 200 µm3 scan range with 50 nm resolution. The experimental results of the 2D magnetic resonance force map carried out on diphenylcyclohexatriene (DPH) at T = 1.1 K are shown and an improvement of the SNR by 154 compared with the results at room temperature is confirmed. The 2D reconstructed images will be as well.

1Presenting Author
C1.00230 High-Resolution Combined Low-Temperature Scanning Tunneling/Atomic Force Microscope for 3D Force Spectroscopy , B.J. ALBERS, M. LIEBMANN, T.C. SCHWENDEMANN, M.Z. BAYKARA, Yale University, M. HEYDE, M. SALMERON, Lawrence Berkeley Nat. Lab., E.T. ALTMAN, U.D. SCHWARZ, Yale University — We present the design and first results from a new home-built low-temperature scanning probe microscope enabling high-resolution experimentation in both scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) modes. A tuning fork based Q-plus style sensor is used to allow for flexibility in choosing probe tip materials. The system features an on-top cryostat, where the microscope is enclosed in a double set of thermal shields. Tip as well as sample can be changed in-situ at low temperatures to keep turn-around times low. By opening the front shutters of the shields, unrestricted access from dedicated flanges permits the direct deposition of molecules or atoms on either tip or sample while they remain cold. As examples for the microscope’s performance, we present data measured on Cu(111) in STM mode as well as on graphite in NC-AFM mode, featuring atomic resolution with corrugations of 4-5 pm and corrugations below 1 pm could be measured. In addition, atomic resolution data obtained by local force spectroscopy is shown.

C1.00231 Using Nuclear Magnetic Resonance Force Microscopy with Cross-Polarization for Nuclear Magnetization Enhancement and Heteronuclear Decoupling1 , ROSA ELIA CÁRDENAS, JOHN T. MARKERT, Department of Physics, University of Texas at Austin — We report our progress in applying Nuclear Magnetic Resonance Force Microscopy (NMRFM) to study position-dependent cross-polarization effects in ammonium hexafluorophosphate (NH4PF6). Cross polarization (CP) is typically used either to enhance the polarization of a weak or rare species, or to decouple one species from its dipolar interactions with another, that is, for line narrowing. With the added local probe abilities of NMRFM, particularly the presence of a strong field gradient, new techniques for coupling spins in nearby resonant slices are possible. The NH4PF6 system has three NMR-active nuclei: the stronger 1H and 19F nuclear moments, and the weaker and more rare 31P moments. We will examine the various effects of coupling 1H and/or 19F with 31P, including efficient frequency-sweep matching for optimization of the CP rate. We will also examine local effects dependent on excitation and detection slice geometry, and the dynamical effects of NH4 and PF6 reorientations.

1This work was supported by NSF Grant No. DMR-0605828.

C1.00232 Tip-Sample Gap control for truly noncontact operation on an AFM , YEHIAM PRIOR, ALEXANDER MILNER, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — A new mode of operation is introduced to standard atomic force microscopes, working under ambient conditions, for noncontact operation at a small predetermined Tip Sample Gap (TSG) of a few nanometers. A phase-locked loop, based on tiny oscillations (<1 nm) of the cantilever at a frequency far from the cantilever mechanical resonances, is used to maintain the gap between the tip and the sample at a range of 1 - 4 nanometers. The noncontact hovering of the tip is maintained for long times without the tip ever touching the surface. The TSG is calibrated by the far field scattering of evanescent fields over transparent samples. A typical measurement run provides, in addition to the standard topography, information about the amplitude and phase of the new oscillations, as well as information about the shear forces based on lateral oscillation of the sample relative to the tip. In a geometry characteristic for Apertureless Scanning Near Field Optical Microscope, the tip is illuminated by a focused beam of a femtosecond laser (800 nm, 20 fs, 100 mw) for nano-patterning of the area under the tip.

C1.00233 A physically founded model of the efficiency curves of coaxial Germanium detectors , YUNXIA GUAN, LIANBIN NIU, YAN MA, JIANZHANG XUE, QING KANG, Department of Physics, Chongqing Normal University — A semi-empirical formula for the full energy peak efficiency of coaxial Germanium detectors in the range of 60 to 2614 keV is presented. Both equations are linear with respect to the fitting parameters. They were obtained by combining, and minor adjusting, the terms in the asymptotic expressions for the probabilities of the processes (photoelectric absorption, Compton Scattering and pair production) through which γ-rays interact with matter. Both equations were found to be able to fit very well in wide energy ranges the efficiency curves of coaxial Ge detectors detecting γ-rays from point or plane sources, as well as from cylindrical volume sources.

C1.00234 Derivation of sensitivity of a Geiger mode APDs detector from a given efficiency to estimate total photon counts , KIYOTAKA HAMMURA, Hitachi Cambridge Laboratory, Cavendish Laboratory, UK — In quantum key distribution (QKD) experiments based on a single photon stream, a single photon detector incorporating Geiger mode avalanche photodiodes (APDs) is mostly used in order to detect photons. It is important to estimate prior to experiments how many photons the detector can detect in total for a simple single photon stream. We propose a method of estimating it using intrinsic detection sensitivity (DS) instead of extrinsic detection efficiency (DE). We derive DS using figures to examine the various effects of coupling H and/or F with P, including efficient frequency-sweep matching for optimization of the CP rate. We will also examine local effects dependent on excitation and detection slice geometry, and the dynamical effects of NH4 and PF6 reorientations.

\[
DS = \frac{\text{How many photons have been counted per second}}{\text{How many photons have arrived per second} - N_B} \quad (1)
\]

resulting in 0.27. Applying this value of DS to our experimental configuration, the total photon counts are estimated at 81,000 counts/second. DE under these configurations is estimated at 0.16, which is found to be smaller than that at a lower triggering rate configuration.

C1.00235 METALS —

C1.00236 ABSTRACT WITHDRAWN —

C1.00237 Dynamic acoustic effects and hysteresis in dislocation-based kinking nonlinear elastic solids under stresses , PETER FINKEL, Drexel University — We argue that proposed recently mechanism explaining inelastic hysteresis in non-linear elastic systems indeed can be explained by means of formation of dislocation-based incipient kink bands (IKB). Using acoustic waves we investigated possible dislocation related mechanisms responsible for nonlinear dynamic response of IKB solids. In this work, for the first time we observed and reversibility of IKB formation directly under stress using ultrasonic waves and acoustic emission signatures during compression test of nanolaminated layered ternary carbide (MAX phases) and hexagonal metal samples. We confirm here that the dynamic behavior of these non-linear elastic systems is due to the interaction of dislocations with the stress waves.
C1.00238 Direct Estimation of Strain Gradient Maps in Plane Strain Indentation. TEJAS MURTHY, CHIHYUNG HUANG, SRINIVASAN CHANDRASEKAR, Purdue University — Indentation is a widely used non-destructive means for assaying mechanical properties of metals. In-situ Experimental investigations on the extent of deformation and the distinct features of the deformation field around a plane strain wedge indenter were performed. A rigid plastic material (lead) was indented under plane strain conditions with different deformation rates and wedge angles. The region around the indenter was directly observed by tracking asperity movements on the surface of the specimen using high-speed imaging. The digitized images were analyzed using particle image velocimetry (PIV) to obtain velocity fields. Strain rate fields and strain maps were also obtained through analysis of this velocity field. Estimates of the strain gradients at a macro scale have afforded detailed analysis of the size effects in indentation and validation of flow theories at a macroscopic scale.

C1.00239 Ab initio simulations of grain boundary sliding in aluminum and nickel. JITESH GARG, Department of Mechanical Engineering, Massachusetts Institute of Technology, NICOLA MARZARI, Department of Materials Science and Engineering, Massachusetts Institute of Technology — The Hall-Petch relationship predicts an increase in material yield strength with decreasing grain size. However, a breakdown has been reported at smaller grain sizes, where plastic deformation gradually becomes grain-boundary dominated. Studying grain-boundary sliding processes is therefore key to understanding the mechanical properties of polycrystalline materials. In the present work, we use density-functional theory to examine the microscopic processes that accompany grain boundary sliding in aluminum and nickel for different grain boundary structures. Sliding of tilt boundaries is also accompanied with grain boundary migration, where grain boundary movement normal to the boundary surface takes place. The effect of adding W to the sliding process in Ni-W alloys is also reported.

C1.00240 Laser induced patterning of metal films via weakly bound layers on surfaces. MICHA ASSCHER, ORI STEIN, YIGAL LILACH, The Hebrew University of Jerusalem, LEONID V. ZHIGILEI, ZHIBIN LIN, University of Virginia, Charlottesville — Pulsed laser heating of weakly binding layers has been employed for selective removal of these layers. The ablated films (Xe) are then used as templates for metallic clusters and film patterning. The method enables patterning over most substrates that absorb the laser light, e.g. Ru(001) single crystal, soft surfaces prepared from self-assembled monolayers (SAM) and SiO$_2$/Si(100). Patterns obtained from interfering laser beams result in a ratio of laser wavelength to width of pattern’s edge less than 1:40, better than most standard optical, mask-less patterning techniques. In-situ optical diffraction has been utilized to study the thermal stability of the patterned weakly bound films against surface diffusivity and desorption. Molecular Dynamics simulations of a Xe film composed of 15,000 atoms attached in 14 layers, has demonstrated a threshold for ablation at 100J/m$^2$. At identical laser energy above threshold and 3-10 ps pulse duration range, longer pulses result in better patterning resolution.

C1.00241 Laser-induced dewetting nanomorphology and nanostructure in immiscible bilayer metal films. H. KRISHNA, Dept. of Physics, Washington University in St. Louis, MO, R. SURESHKUMAR, Dept. of Energy, Environmental and Chemical Engineering, Washington University in St. Louis, MO, R. KALYANARAMAN, Dept. of Physics, Washington University in St. Louis, MO — Spatially ordered patterns of nanoparticles result under ns laser-induced dewetting of immiscible bilayer metallic films (Co and Ag) on inert substrates like SiO$_2$. The morphological pathway during dewetting is different for the two individual metals: occurring through development of bicontinuous structures in the case of Ag and by progression of cellular networks for Co. On the other hand, dewetting in bilayer structures of Ag/Co/SiO$_2$ or Co/Ag/SiO$_2$ shows that the morphology evolution is dictated by the thicker of the two films. Linear stability analysis predicts that the self-organized length scales from the bilayer film dewetting is smaller than a single layer of either metal with the same total thickness. This was also verified experimentally and shows that the metal-metal interfacial dynamics significantly influences bilayer dewetting. Electron microscopy investigations show that the individual nanoparticles consist of Ag and Co in their individual elemental crystal phase. These ns laser dewetting experiments provide novel ways to create multi-metal patterns and nanostructures.

C1.00242 An Evaluation of the Rigid Band Model and the Virtual Crystal Approximation in the Transition Metals. DIMITRIOS PAPACONSTANTOPOULOS, FRED IACOLETTI, ALEX KOUFOS, George Mason University — The Schrodinger equation was solved using the Augmented Plane Wave (APW) Method for transition metals in both the body centered cubic (bcc) and face centered cubic (fcc) structures. This method accurately predicts the equilibrium lattice parameter and the ground state of all transition metals. The Rigid Band Model tests based on the group eight and group nine transition metals was applied to predict the density of states (DOS) at the Fermi level for the rest of the transition metals. This test agreed with direct calculations quite well with only a few exceptions in the hexagonal structures. The APW method was also applied using the virtual crystal approximation to obtain the DOS of binary alloys. The results will be compared with direct calculations of ordered and disordered structures.

C1.00243 The Density Functional Calculation for Surface Capacitance of Metal-Semiconductor Junction. CHIN-SHENG WU, Yuan Ze University — We use the density functional theory to find the density of the surface electronic charge around metal-semiconductor junction. We use the local approximation for the inhomogeneous dielectric function around the junction. Therefore this surface charge can be applied to find dielectric constant, which is a function of the electron density. The capacitances are calculated on the junction by their shapes and dielectric constants for various metal and semiconductor densities.

C1.00244 Comparison of the Phase Field Crystal Free Energy Functional and the Second Order Density Functional Theory of Freezing. AKUSTI JAATINEN, CRISTIAN ACHIM, JARI JALKANEN, TAPIO ALA-NISSILA, Laboratory of Physics, Helsinki University of Technology, Espoo, Finland, KEN ELDER, Department of Physics, Oakland University, Rochester, Michigan, USA — We present a numerical study of the recently established connection between the phenomenological free energy functional of the phase field crystal model (PFC) and the second-order density functional theory of freezing (DFT) [1]. We have used liquid state structural data of iron and copper near their melting points to study their freezing properties by both DFT and PFC functionals. The results obtained by the two functionals differ from each other significantly. DFT being superior to PFC in predicting crystal structures, density profiles and coexistence densities. We conclude that the fitting procedure outlined in [1] does not provide quantitatively accurate predictions of phase diagrams. [1] K. R. Elder, N. Provatias, J. Berry, P. Stefanovic and M. Grant, Phys. Rev. B 75, 064107 (2007)

C1.00245 ABSTRACT WITHDRAWN

C1.00246 STATISTICAL AND NONLINEAR PHYSICS
Doebner-Goldin Equation for Electrodynamic Model Particle & Applications

J.X. ZHENG-JOHANSSON — We set up based on Maxwell’s equations the classical wave equation for the total wave of a particle composed of an oscillatory charge of zero rest mass and the resulting electromagnetic waves traveling in the force field of an usual potential and an additional fractional force \( f \). The equation decomposes into a component equation describing the particle kinetic motion, which for \( f = 0 \) identifies with the usual Schrödinger equation. The \( f \)-dependent probability density presents generally an observable diffusion current of a real diffusion constant; this and the particle’s usual quantum diffusion current as a whole are under adiabatic condition conserved and obey the Fokker-Planck equation. The extra, \( f \)-dependent Hamiltonian operator identifies with that obtained by Doebner and Goldin. The friction produces to the particle’s wave amplitude a damping that can describe well the effect due to a radiation (de)polarization (RD) field, which is always by-produced by the particle’s oscillatory charge in a (nonpolar) dielectric medium; such a friction and the resulting observable diffusion as intrinsically accompanying the particle motion was as strikingly conjectured in the Doebner and Goldin original discussion. The RD field in a dielectric vacuum exerts on another particle an attractive, depolarization radiation force which on the whole resembles Newton’s gravity, and on the particle itself an attractive, self depolarization radiation force whose time rate gives directly the \( f \) (full paper: SNMP2007).

C0.00248 The Effects of Popping Popcorn Under Reduced Pressure

PAUL QUINN, AMANDA COOPER, Kutztown University — In our experiments, we model the popping of popcorn as an adiabatic process and develop a process for improving the efficiency of popcorn production. By lowering the pressure of the popcorn during the popping process, we induce an increase in popcorn size, while decreasing the number of remaining unpopped kernels. In this project we run numerous experiments using three of the most common popping devices, a movie popcorn maker, a stove pot, and a microwave. We specifically examine the effects of varying the pressure on total sample size, flake size and waste. An empirical relationship is found between these variables and the pressure.

1Thanks to the students of the New Jersey Governor’s School of the Sciences for assistance in carrying out portions of this project.

C0.00249 Dynamic localization and transport of a quantum particle in an optical lattice.

PANAGIOTIS MANIADIS, Los Alamos National Laboratory, Los Alamos NM, GEORGE P. TSIRONIS, Department of Physics and FORTH, University of Crete, Greece — We study the localization and the transport of a quantum particle in an optical lattice under the influence of an AC electric field. For the description of the particle we use a generalized Discrete Nonlinear Schrödinger equation with local and nonlocal nonlinearities Depending on the parameters of the system, and the external driving field, different behavior is observed (hopping, diffusion, dynamic localization). We explore numerically the behavior of the particle for different values of the external field and the internal nonlinearity parameters, and we compare our results with experimental observations.

C0.00250 Hysteresis-induced long-time tails

GUENTER RADONS, Institute of Physics, Chemnitz University of Technology — Many systems ranging from magnetic materials to shape memory alloys, or fluids in porous structures show complex hysteretic behavior in the sense that besides major loops, subloops and non-local memory effects are observed. The most prominent phenomenological model to account for such effects is the so-called Preisach model [1]. For this model it is shown analytically that uncorrelated input in time is transformed into output showing power-law decay of correlations and 1/f-noise. The characteristic exponents are shown to depend on the tails of the input density and the Preisach density. Universality classes leading to these results are identified.


C0.00251 Reaction-Diffusion Processes on Networks

KYUNSGIK KIM, Department of Physics, Pukyong National University, Pusan 608-737, Korea, SOO YONG KIM, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea, KI-HO CHANG, Global Environment System Research Laboratory, National Institute of Meteorological Research, KMA, Seoul 156-720, Korea — We study the novel reaction-diffusion process of three-species on scale-free networks, which is significantly different from the numerical calculation manipulated on regular and small-world lattices. The inverse particle density for three-species process scales as the power-law behavior with \( \alpha = 1.5 \) for \( \gamma > 3 \). However we find that the inverse particle density scales in a different way depending on time \( t \) when \( \gamma < 3 \). In the early time regime, \( \alpha \simeq 1.5 \) but the inverse particle density increases exponentially as time increases. We also discuss the possible relationship to the dynamical properties of random walks. Particularly, we measure the ratio between the number of inactive and active bonds which shows the segregation of the particles.

C0.00252 A node-weight description on a kind of cooperation-competition networks

DAN SHEN, DA-REN HE, Yangzhou University — Cooperation and competition between elements usually appear together in complex systems. We consider the kind of the systems, which can be described by bipartite graphs. In the networks there are two types of nodes: some activities, organizations or events, and the participators. The traditional bipartite graph statistical properties may describe the configuration of the cooperation-competition, and the statistical properties about a node weight may describe the different role of a node in cooperation or competition result. We shall present some empirical investigations on Chinese Movie Network, Beijing Restaurant Network and IT product Network as examples.

1supported by the National Natural Science Foundation of China under the key project Grant No. 10635040 and the Grant No. 70371071

C0.00253 IT product competition Network

XIULI-LIAN XU, LEI ZHOU, JIAN-JUN SHI, YONG-LI WANG, AI-XIA FENG, DA-REN HE, Yangzhou university — Along with the technical development, the IT product competition becomes increasingly fierce in recent years. The factories, which produce the same IT product, have to improve continuously their own product quality for taking a large piece of cake in the product sale market. We suggest using a complex network description for the IT product competition. In the network the factories are defined as nodes, and two nodes are connected by a link if they produce a common IT product. The edge represents the sale competition relationship. 2121 factories and 265 products have been investigated. Some statistical properties, such as the degree distribution, node strength distribution, assortativity, and node degree correlation have been empirically obtained.

1supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C0.00254 The combined traffic network of China

CHANG-GUI GU, SI-JUN PAN, KAI-JUN LI, YAN-QING QU, CHAO QIAO, YU-MEI JIANG, DA-REN HE, Yangzhou University — From a new viewpoint, we study the combined traffic network of china including the intercity bus network, the railway network, and the airplane network. Some statistical properties, such as averaged distance, clustering coefficient, assortativity, degree distribution, and degree correlation have been empirically investigated for each traffic network and the combined one. From the results we found that the cumulative distribution of cluster coefficient is in a good agreement with the node degree distribution. In order to describe the jumping between the sub-networks, we define and discuss some new statistical properties, such as the jump-convenience and average jumping distance. This may be the first investigation on a combined traffic network.

1supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089
from the fully developed turbulence. The simple binomial multiplicative process is not appropriate to catch its dynamics. It means that the market information process can be essentially different order correlations between successive pieces of market information. Although the multifractal properties of the market information process is clearly confirmed, the context of two-phase phenomenon is introduced in financial exchange markets. To find the underlying process of the formation of market information, we

LEE, Department of Environmental Atmospheric Science, Pukyong National University, Pusan 608-737, Korea — The market information and its intensity for

Quantifying these correlations we especially find triangle- and 3-star-motifs to correlate with one another. Markov Chain Monte Carlo simulations confirm the

networks with triangle- and 3-star-type interaction among bi-valued edges. We discuss the analytical expressions for the statistics' averages in mean-field

Urbana-Champaign, NOSHIR CONTRACTOR, IEMS, Northwestern University — We study the equilibrium statistical mechanics of ensembles of undirected

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probability of secreting the same mediators by all neuroendocrine cells, is observed as s=0.14. Our results may be used in the research of the medical treatment

act degree of neuroendocrine network is h=3.01, It means that each mediator is secreted by three cells on average. The similarity, which stands for the average

bodily healthiness, emotional stabilization and endocrine harmony. The act degree distribution shows a shifted power law (SPL) function forms [1]. The average

the most important mitogenic cytokine, followed by TGF-beta, IL-6, IL1-beta, VEGF, IGF-1and so on. They are critical in neuroendocrine system to maintain

stands for the number of the cells that secrete a single mediator. Among them bFGF (the basic fibroblast growth factor) has the largest node act degree. It is

it by a bipartite graph. In the net the cells can be regarded as collaboration acts and the mediators can be regarded as collaboration actors. The act degree

The node weight usually signify the role or “importance degree” of each actor. We propose using some statistical properties for the description of such kind of systems. The properties without considering node-weight can describe the cooperation situation and configuration. The properties with node-weight considered may describe the competition results. We report an example system, the fruit nutritive factor network, to show the description method and the corresponding empirical investigation results. It is our wish that the description method could be widely effective for the kind of systems in variety different scientific fields.

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00255 A network description on fruit nutritive factor system1, YAN-QING QU, YU-MEI JIANG, DA-REN HE, Yangzhou University — We propose describing a kind of cooperation-competition systems by node-weighted bipartite graphs. In the systems the nodes can be divided into two types. One type expresses a kind of activities, organizations or events, named “acts”; the other expresses the “actors” participating the acts. In each act the actors basically show collaboration relationship, however they play different role in the cooperation. This is a kind of competition. The node weights usually signify the role or “importance degree” of each actor. We propose using some statistical properties for the description of such kind of systems. The properties without considering node-weight can describe the cooperation situation and configuration. The properties with node-weight considered may describe the competition results. We report an example system, the fruit nutritive factor network, to show the description method and the corresponding empirical investigation results. It is our wish that the description method could be widely effective for the kind of systems in variety different scientific fields.

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00257 A Collaboration Network Model Of Cytokine-Protein Network1, SHENG-RONG ZOU, TA ZHOU, YU-JING PENG, ZHONG-GUI GUO, CHANG-GUI GU, DA-REN HE, Yangzhou University — Complex networks provide us a new view for investigation of immune systems. We collect data through STRING database and present a network description with cooperation network model. The cytokine-protein network model we consider is constituted by two kinds of nodes, one is immune cytokine types which can be regarded as collaboration acts, the other one is protein type which can be regarded as collaboration actors. From act degree distribution that can be well described by typical SPL (shifted power law) functions [1], we find that HRA, TNFSF13C, S100A8, S100A1, MAPKI, S100A7, LIF, CCL4, CXCL13 are highly collaborated with other proteins. It reveals that these mediators are important in cytokine-protein network to regulate immune activity. Dyad in the collaboration networks can be defined as two proteins and they appear in one cytokine collaboration relationship. The dyad act degree distribution can also be well described by typical SPL functions. [1] Assortativity and act degree distribution of some collaboration networks, Hui Chang, Bei-Bei Su, Yue-Ping Zhou, Daren He, Physica A, 383 (2007) 687-702

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00258 An Empirical Study of Immune System Based On Bipartite Graphs1, YU-JING PENG, SHENG-RONG ZOU, ZHONG-GUI GUO, TA ZHOU, CHANG-GUI GU, DA-REN HE, Yangzhou University — Immune system is the most important defense system to resist human pathogens. We present an immune bipartite graph model. Firstly we collect data through COPE database and then construct an immune cell-mediator network. In the net the immune cells can be regarded as collaboration acts and the mediators can be regarded as collaboration actors. The act degree distribution of this network is proved to be power-law with a scaling exponent 1.8. From our analysis, we found that some mediators with high degree are very important in the process of regulating immune activity, such as TNF-alpha, IL-8, TNF-alpha receptors, CCL5, IL-6, IL-2 receptors, TNF-beta receptors, TNF-beta, IL-4 receptors, IL-1 beta, CD54 and so on. We also found that the assortativity coefficient of the immune network is -0.27.

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00259 A bipartite graph of Neuroendocrine System1, ZHONG-GUI GUO, SHENG-RONG ZOU, YU-JING PENG, TA ZHOU, CHANG-GUI GU, DA-REN HE, Yangzhou University — We present an empirical investigation on the neuroendocrine system and suggest describe it by a bipartite graph. In the net the cells can be regarded as collaboration acts and the mediators can be regarded as collaboration actors. The act degree stands for the number of the cells that secrete a single mediator. Among them bFGF (the basic fibroblast growth factor) has the largest node act degree. It is the most important mitogenic cytokine, followed by TGF-beta, IL-6, ILL1-beta, VEGF, IGF-1and so on. They are critical in neuroendocrine system to maintain bodily healthiness, emotional stabilization and endocrine harmony. The act degree distribution shows a shifted power law (SPL) function forms [1]. The average act degree of neuroendocrine network is h=3.01. It means that each mediator is secreted by three cells on average. The similarity, which stands for the average probability of secreting the same mediators by all neuroendocrine cells, is observed as s=0.14. Our results may be used in the research of the medical treatment of neuroendocrine diseases. [1] Assortativity and act degree distribution of some collaboration networks, Hui Chang, Bei-Bei Su, Yue-Ping Zhou, Daren He, Physica A, 383 (2007) 687-702

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00260 Triangle-3star-Correlations in the mean-field solution of equilibrium ensembles of undirected networks with 3-edge interactions, PETER FLECK, Center for Complex Systems Research, University of Illinois at Urbana-Champaign, NOSHIR CONTRACTOR, IEMS, Northwestern University — We study the equilibrium statistical mechanics of ensembles of undirected networks with triangle- and 3-star-type interaction among bi-valued edges. We discuss the analytical expressions for the statistics' averages in mean-field approximation as a function of these interaction parameters. We find these averages to be highly correlated for a large region of the parameter space. Quantifying these correlations we especially find triangle- and 3-star-motifs to correlate with one another. Markov Chain Monte Carlo simulations confirm the analytical mean-field results in an important part of parameter space. Implications for the analysis of network topologies are being discussed.

C1.00261 Multifractal Behaviors in Foreign Exchange Markets, KYUNGSIK KIM, Department of Physics, Pukyong National University, Pusan 608-737, Korea — The market information process can be essentially different from the fully developed turbulence.

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089
C1.00262 Universality in rank distributions due to multiplicative processes: from power laws to stretched exponentials. GERARDO NAUMIS, Depto. de Física-Química, Instituto de Física, UNAM, GERMINAL COCHO, Instituto de Física, SISTEMAS COMPLEJOS-FISICA-QUIMICA COLABORATION — Although power laws have been used to fit rank distributions in many different contexts, they usually fail at the tails. Stretched exponentials and log-normal distributions have been used to solve the problem, but unfortunately they are not able to fit at the same time both ending tails. Here we show that many different data in rank laws, like in granular materials, codons, author impact in scientific journal, etc. are very well fitted by a beta-like function (a,b distribution). Since this distribution is indeed ubiquitous, it is reasonable to associate it to the product of correlated probability distributions. In particular, we have found that the macrostates of the product of discrete probability distributions imply stretched exponential-like frequency-rank functions, which qualitatively and quantitatively can be fitted with the a,b distribution in the limit of many random variables [1]. We prove this by transforming the problem into an algebraic one: finding the rank of successive products of a given set of numbers. [1] New J. Phys. 9 (2007) 286. (2007).

C1.00263 Dynamical Behaviors of rainfalls in Korean peninsula. KYUNGSIK KIM, Department of Physics, Pukyong National University, Pusan 608-737, Korea, SOO YONG KIM, GYUCHANG LIM, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea, KI-HO CHANG, JAE-WON JUNG, Global Environment System Research Laboratory, National Institute of Meteorological Research, KMA, Seoul 156-720, Korea, SANG-BUM PARK, Department of Business Administration, Hankuk Aviation University, Goyang 412-791, Korea, MYUNG-KUL YUM, Department of Pediatric Cardiology, Hanyang University, Kuri 471-701, Korea — Application of ideas from fractal and chaos theories to characterize rainfall is one of the most active and exciting areas of research in this field. Many studies performed thus far have yielded evidence of the existence of fractal and chaos properties in rainfall. In this work, we present a singularity spectrum of a rainfall time series to provide strong evidence of multifractality. A curdling cascade process in a well developed turbulence is considered as a candidate to describe the rainfall, and the analogy between the rainfall and turbulence is confirmed via the validity of the binomial multiplicative process to describe both systems.

C1.00264 Colloids in a periodic potential: driven lattice gas in continuous space, RONALD DICKMAN, UFMG, FABRICIO POTIGUAR — Motivated by recent studies of colloidal particles in optical tweezer arrays, we study a two-dimensional model of a colloidal suspension in a periodic potential. The particles are confined to stay near potential minima, approximating a lattice gas. The interparticle interaction, a sum of Yukawa terms, features short-range repulsion and attraction at somewhat larger separations, such that two particles cannot occupy the same potential well, but occupation of adjacent cells is energetically favored. Monte Carlo simulation reveals that the equilibrium system exhibits condensation, as in the Ising model/lattice gas with conserved magnetization; the transition appears to be continuous at half occupancy. We study the effect of biased hopping, favoring motion along one lattice direction. This system is found to exhibit features of the driven lattice gas: the interface is oriented along the drive, and appears to be smooth. A weak drive facilitates ordering of the particles into high- and low-density regions, while stronger bias tends to destroy order, and leads to very large energy fluctuations. We also study ordering in a moving periodic potential. Our results suggest possible realizations of equilibrium and driven lattice gases in a colloidal suspension subject to an optical tweezer array.

C1.00265 Disordered contact process in two and three dimensions: rare regions, Griffiths effects, and infinite randomness, ADAM FARQUHAR, JASON MAST, THOMAS VOJTA, University of Missouri-Rolla — We investigate the effects of quenched spatial disorder on the directed percolation universality class in two and three space dimensions. To this end we perform large-scale Monte-Carlo simulations of the contact process on a randomly diluted lattice for times up to $10^{10}$ and system sizes up to $6 \times 10^3$ sites. We study both the nonequilibrium phase transition and the associated Griffiths region between the clean and disordered critical points. Rare strongly coupled regions lead to slow dynamics characterized by a nonuniversal power-law density decay in the entire Griffith region. In two dimensions, we also perform a detailed scaling analysis of the critical behavior right at the phase transition. We find an infinite-randomness critical point with activated rather than power-law dynamical scaling. However, the critical region is narrow and the approach to the asymptotic dynamics is extremely slow, which hampers the precision of our critical exponent estimates. We discuss the generality of our findings and relate them to a broader theory of rare region effects at phase transitions with quenched disorder.

C1.00266 Phase diagram, depinning and sliding friction in the Phase Field Crystal model. TAPIO ALA-NISSILA, CRISTIAN BASILE ACHIM, Helsinki University of Technology, Laboratory of Physics, Espoo, Finland, KEN R. ELDER, Oakland University, Department of Physics, Rochester, United States, MIKKO KARTTUNEN, The University of Western Ontario, Department Of Applied Mathematics, London, Canada, ENZO GRANATO, Instituto Nacional de Pesquisas Espaciais, Laboratório Associado de Sensores e Materiais, São José dos Campos, Brazil, SEE CHEN YING, Brown University, Department of Physics, Providence, United States — We present results for commensurate-incommensurate transitions and non-linear sliding friction for a two-dimensional crystal lattice in the presence of an external pinning potential in the Phase Field Crystal model. This model provides a continuum description of lattice system, such as adsorbed monolayers or two-dimensional vortex lattice. The competition between the length scales associated with the intrinsic ordering and the pinning potential leads to commensurate-incommensurate transitions. The dynamical response of the system in the presence of a driving force has also been studied via the time dependent Ginzburg-Landau equation. We present results on non-linear dynamics and sliding mechanisms for commensurate phases.

C1.00267 Development of a Fracture Network: blocks and springs model, MARTIN FERER, ADAM JOZWICK, Physics, West Virginia University, DUANE SMITH, U.S., D. O. E., National Energy Technology Laboratory — Since flow in fractured reservoirs is significantly enhanced by clusters of inter-connecting fractures, it's important to understand their inter-connectedness. In these fractured reservoirs, one often finds two sets of fractures: the primary and secondary fractures. The secondary fractures intersect the first generation of. We find a percolation-like transition where the cluster size grows with increasing strain leading to system-spanning fractal clusters. Increasing the thickness of the layer being fractured leads to sparser system-spanning fracture clusters with smaller fractal dimension. We have studied how the thickness of the layer affects the fractal character of the fracture clusters as well as their number distribution, and the correlations within the large fracture cluster.

C1.00268 Cyclic deformation of polymer glasses in the yield regime by a contact method. ANTOINE CHATEAUMINOIS, CHRISTIAN FREITIGNY, ESPCI — Cyclic strains in the yield regime are characterized by a slow evolution of the mechanical response of polymer glasses toward a poorly understood stationary state. In this study, the dynamics of plastically deformed polymer glasses is analysed by a contact method where a thin film is geometrically confined and sheared within a contact between two elastic substrates. As opposed to conventional mechanical testing using bulk polymers, this approach allows to investigate the cyclic plastic behavior without the complications arising from fracture. From a measurement of the lateral contact response, we have shown that the shear properties of the film can be determined both in the linear and in the non linear regime. Using this approach, the time and strain dependent shear response of polymer glasses in the yield regime will be discussed. In addition, linear viscoelastic measurements carried out after the application of cyclic yield provides information about the dynamics of plastically deformed glass and its recovery.

This work is supported by CNPq and Faperj, Brazil.
C1.00260 Numerical studies of the Zaitsev (Robin Hood) model, PERRY FOX, GABRIEL CWILICH, SERGEY BULDYREV, FREDY ZYPMAN. Department of Physics - Yeshiva University — The Zaitsev[1] model of depinning of interfaces has been widely used to discuss motion of dislocations, low temperature flux creep, and more recently dry friction. The properties of this model have been discussed theoretically in one dimension, and numerically verified with precision in the isotropic case. We are studying here the effect of anisotropy in the distribution of the “mass” among the neighbors in the updating of the sites, which is known to modify the critical exponents of the model in one dimension. We have considered the validity of the scaling laws in higher dimensions, which might be relevant for the case of friction [2], by computing several of the exponents of the model for the avalanche size distribution, avalanche fractal dimension and distribution of jumps between external sites of activity. The much richer space of parameters of anisotropy in two dimensions has been explored. [1] S.I. Zaitsev, Physica A189, 411 (1992). [2] S. Buldyrev, J. Ferrante and F. Zypman Phys. Rev E64, 066110, (2006)

C1.00270 A physical mechanism for enhanced orientational order of self propelled hard rods, APARNA BASKARAN, CRISTINA MARCHETTI. Syracuse University — We consider a model of 2D hard rods on a substrate. The rods interact through energy and momentum conserving binary collisions. Self propulsion is implemented as a center of mass force acting along the long axis of each rod. The nonequilibrium statistical mechanics for this microscopic model is systematically developed. In the overdamped regime, the dynamics is described by a modified Smoluchowski equation that includes new momentum transfer contributions that arise from self propulsion. Hydrodynamic equations for the density, polarizability and nematic order parameter are derived by coarse graining the Smoluchowski equation. The homogeneous equations yield an isotropic-nematic transition at lower densities than the Onsager density corresponding to an equilibrium system of hard rods. This enhanced ordering arises from the additional momentum transfer associated with self propulsion and is expected to be a generic feature of a broad class of active systems.

C1.00271 Statistics preserving formation of chaotic swarmers, IULIANA OPREA, Colorado State University, IOANA TRIANDAF, IRA SCHWARTZ, Naval Research Laboratory — We present a class of models for self-propelled multi-agent systems of autonomous vehicles that accomplish common tasks while preserving the formation moments of inertia. The models are based on simple, local interaction rules that create prescribed overall complex patterns in which coupling and communication are key elements. We use a statistics-preserving algorithm with a Duffing-like term added to the equations of motion to control the moments of the pattern formation. We concentrate on those parameters in the neighborhood of a resonant situation. This allows us to obtain interesting patterns of behavior similar to those observed in parametrically forced systems near resonance.

1Work supported by the Office of Naval Research.

C1.00272 Modular Networks in the Neocortex, H.G.E. HENTSCHEL, Emory University — We will describe our approaches to characterizing the network architecture of active neurons in mouse neocortex in terms of modules and functional motifs, in order to extract their information processing capabilities. The raw data comes from fast two photon microscopic techniques recently developed using fluorescent Ca2+ indicators to record the spontaneous and evoked activity from hundreds of identified cells in mouse. This ensemble of active neurons can be considered as a complex network linked by synaptic connections, and represented as a graph of nodes connected by edges. Information processing in the network requires interaction of neurons in different functional assemblies (microcircuits) over time. We will describe the information we have been able to uncover on these microcircuits and their function.

C1.00273 Study on the hierarchical property between the functional classes in protein-protein interaction network, YOUNG-JIN KO, SOON-HYUNG YOOK, YUP KIM, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Detecting community structures and hierarchy among communities have been one of the most attractive research topics in complex network studies. In this study we regard each protein as an oscillator which interacts with its neighboring proteins. In order to define the hierarchy among the functional classes based on the synchronizability of each functional classes, we introduce a parameter $r_{\text{link}}$. Here $r_{\text{link}}$ represents the fraction of all possible links whose ends nodes are synchronized. From the numerical simulations we find that the hierarchical structure between functional classes does not depend on the coupling strength. We expect that this result provides a clue to understand the mechanism to form the specific structure of PIN. Some possible relationships between the observed hierarchical structure of the functional classes and the properties of the PIN are also discussed.

C1.00274 Phase synchronization induced by common external telegraphic noise, KEN NAGAI, Kyoto University — Generally, noise desynchronizes phase of nonlinear oscillators. However, when a neuron receives a randomly fluctuating input current, its reliability of spike generation improves compared with the case of a constant input current [Mainen and Sejnowski, Science 268, 1503 (1995)]. Like this phenomenon, phase synchronization between uncoupled nonlinear oscillators subject to a common external noise occurs in some systems. Phase synchronization between uncoupled limit-cycle oscillators is induced by common external telegraphic noise that jumps between two values randomly [Nagai and Nakao, Phys. Rev. E, 71, 036217 (2005)]. We observed this phenomenon with an electric circuit and analyzed it. When the switching time of the input current is sufficiently long, the internal state of the oscillator randomly jumps between two limit cycles corresponding to the input values, which can be described by random phase maps. We determined the phase maps experimentally and discussed the synchronization of oscillators subject to fluctuating inputs, using this maps. The Lyapunov exponents of the maps corresponded to damping rate of the variance of the phase.

C1.00275 Thin-film morphology dependence on adatom-substrate interaction energy, NUNO A.M. ARAUJO, GCEP-Centro de Fisica da Universidade do Minho, 4710 Braga, Portugal; T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; CRISTOVAO S. DIAS, GCEP-Centro de Fisica da Universidade do Minho, 4710 Braga, Portugal, ANTONIO CADILHE, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA. — The influence of adatom-substrate interaction energy on the morphology of heteroepitaxial film growth. We take the case of (1+1)-dimensions for sake of simplicity. We also define $\alpha$ as the quotient between the above interaction and the adatom-adatom interaction. We measure the roughness in time. We show that changing the value of $\alpha$ it is possible to range from a wetting regime to a non-wetting one. We also show that above a critical thickness, film growth becomes independent of adatom-substrate interaction.

C1.00276 Agent based spin model for financial markets on regular lattices and complex networks, HONG-JOO KIM, SOON-HYUNG YOOK, YUP KIM, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — We study an agent based microscopic model for price formation in financial markets on various topologies motivated by the dynamics of agents. The model consists of interacting agents (spins) with local and global couplings. The local interaction denotes the tendency of agents to make the same decision with their interacting partners. On the other hand, the global coupling to the self-generating field represents the process which maximizes the profit of each agent. In order to incorporate more realistic situations, we also introduce an external field which changes in time. This time-varying external field represents any internal or external interference in the dynamics of the market. For the proper choice of model parameters, the competition between the interactions causes an intermittency dynamics and we find that the distribution of logarithmic return of price follows a power-law.
C1.00277 Complexity and Ability in Ising Games, Ayax Ramirez, Southwestern College, Michael George, Southwestern College - In previous work [1, 2], we discussed various facets of designs in games, and considered the evolution [2] of Ising games. The traditional aspect of game theory, with its focus on rational decisions, was not considered in this work. Instead, there was a predominant interest in the time evolution of design toward a goal, and resulting levels of frustration. There was also a concern with time-reversal of meaningfulness. In the new work, our goal is to consider the "molecular structure" of the Ising model as it evolves, and to associate this molecular structure with feedback into the structure that can be understood in algorithmic terms. We develop an analogy with the famous Maltesian argument concerning exponential population increase, associating ability to cope with complexity, and algorithmic complexity, and discuss biological implications of the ideas associated with these games. [1] M. George, A nonequilibrium statistical model based on latin squares, paper presented at WorldComp'07, Las Vegas, Nevada, June 25-28, 2007. [2] M. George, Classical and quantum Ising games, paper presented at Fourth International Conference in Applied Mathematics and Computing, Plovdiv, Bulgaria, August, 2007.

C1.00278 Wrinkled induced by poking a free-floating film under tension1, Narayan Menon, Jiangshui Huang, Dept of Physics, UMass Amherst. Enrique Cerdá, Universidad de Santiago de Chile, Wim De Jeu, Thomas Russell, Dept of Polymer Science, UMass Amherst - We study experimentally and theoretically the out-of-plane deformation in a floating polystyrene film induced by depressing the centre of the film by a distance, d. When this depth exceeds a critical value d_c, the smooth conical deformation of the film becomes unstable to an elastic e^-w-term expansion: d < d_c. Changes; only digit-integer-differences=quanta! Quo vadis digit

C1.00279 Percolation density profiles and lattice structures, Robert Ziff, University of Michigan, Peter Kleban, University of Maine, Jacob Simmons, Oxford University, Christian Scullard, University of Chicago - This paper presents a visual display of results on percolation density profiles from anchor points and intervals along the side, demonstrating our theoretical predictions of various forms of factorization of the three point functions into products of two-point functions (some with square roots). We also show a gallery of numerous lattice structures where the percolation threshold can be found exactly through the triangle-triangle transformation, or approximately (to very high precision) by generalizations of known formulas. Studies of various classes of lattices shows slight but non-zero corrections for most non-triangular configurations. Methods to numerically find the threshold (null generation, cluster growth, and cluster-coalescence) are also presented.


C1.00282 Beijing restaurant network1, Chun-Hua Fu, Pei-Fang Zhnag, Yong-Li Wang, Jian-Jun Shi, Ai-Xia Fang, Da-Ren He, Yangzhou University — We have empirically studied the restaurants in Beijing and suggested a network description on the system. We define the restaurants as nodes and connect a link between two nodes if the two restaurants sell a common dish. The edge represents the sale competition relationship. In order to describe the competition, we define a node weight, which is the mark given by consumers on an evaluation network (http://www.dianping.com), to restaurants as nodes and connect a link between two nodes if the two restaurants sell a common dish. The edge represents the sale competition relationship. We find that both the total node weight, which is defined as the sum of the node weight in all the dishes, and the so-called dish weight, which is defined as the sum of the node weight in one dish, show a rather nice power law distribution.

1 supported by Chinese National Natural Science Foundation, No. 10635040 and 70671089

C1.00283 PHASE TRANSITIONS AND STRONGLY CORRELATED SYSTEMS
C1.00284 Adsorption and Dissociation of Molecular Oxygen on the (0001) Surface of Double Hexagonal Close Packed Americium, PRATIK DHOLABHAI, RAYMOND ATTA-FYNN, ASOK RAY, The University of Texas at Arlington — Oxygen molecule adsorption on (0001) surface of double hexagonal packed americium has been studied in detail within the framework of density functional theory using a full-potential all-electron linearized augmented plane wave plus local orbitals method. The most stable configuration corresponded to molecular dissociation with the oxygen atoms occupying neighboring three-fold hollow h sites. Chemisorption energies and adsorption geometries for the adsorbed species, and change in work functions, magnetic moments, partial charges inside muffin-tins, difference charge density distributions and density of states for the bare Am slab and the Am slab after adsorption of the oxygen molecule will be discussed. The effects of chemisorption on Am 5f electron localization-de-localization in the vicinity of the Fermi level and the reaction barrier calculation for the dissociation of oxygen molecule to the most stable h sites will be discussed.

This work is supported by the U. S. Department of Energy and the Welch Foundation, Houston, Texas.

C1.00285 Mott transition studied by cellular dynamical mean field theory, YUZHONG ZHANG, Johann Wolfgang Goethe-Universität, Institut für Theoretische Physik, MASATOSHI IMADA, Department of Applied Physics, School of Engineering, University of Tokyo, CLAUDIUS GROS, ROSE VALENTI, Johann Wolfgang Goethe-Universität, Institut für Theoretische Physik — We study metal-insulator transitions between Mott insulators and metals. The transition mechanism completely different from the original dynamical mean field theory (DMFT) emerges from a cluster extension of it. A consistent picture suggests that the quasiparticle weight $Z$ remains nonzero through metals and suddenly jumps to zero at the transition, while the gap opens continuously in the insulators. This is in contrast with the original DMFT, where $Z$ continuously vanishes but the gap opens discontinuously.

The present results arise from electron delocalization in momentum space agree with recent puzzling bulk-sensitive experiments on CaV$_3$O$_7$ and SrVO$_3$. Details of the mechanism of Mott transition is studied through doublon-doublon, doublon-holon and spin-spin dynamical susceptibilities.

C1.00286 Pressure Induced Metallization In ACrO$_3$ Perovskite Compounds, CHANGQING JIN, L.X. YANG, Y.W. LONG, Institute of Physics, Chinese Academy of Sciences, Beijing, China, H.Z. LIU, G.Y. SHEN, H.K. MAO, HPCAT at Advanced Photon Source, Argonne National Lab, USA, J.S. ZHOU, J.B. GOODENOUGH, Texas Materials Institute, University of Texas at Austin, USA — We have studied the electrical conductivity and magnetic susceptibility of ACrO$_3$ (A = alkaline earth) perovskites performed at various pressures up to 60 GPa using diamond anvil cell techniques. The samples were synthesized under high pressure high temperatures. Pressure induced metallizations were observed in both samples. However, the x-ray diffraction experiments with resonant radiation source indicated no discernable crystal structural transition up to 60 GPa. Therefore the pressure induced metallizations were ascribed to electronic type phase transitions. It possibly came from the change of electronic structure due to an orbital ordering evolution induced by pressure.

C1.00287 Ultrasonic Study of the Yb-based Heavy Fermion Compound YbCo$_2$Zn$_{30}$, YOSHIKICANAKISHI, Iwate University — We present experimental results of elastic constants as a function of temperature and magnetic field performed on a single crystal of the Yb-based heavy fermion system YbCo$_2$Zn$_{30}$. A marked elastic softening toward low temperature was observed in a longitudinal elastic constant C11 and transverse ones (C11-C11)/2, C44. The softening is suppressed unexpectedly in a weak applied field of 2 T. Our results strongly suggest a large degeneracy of a 4f state of the Yb ion at low temperature and the Heavy Fermion state is quenched by the applied weak field. Thus, it is expected that this highly degenerated situation due to the almost spherical CEF, realized by the unique crystal structure, would form such a heavy fermion state and a lift of the degeneracy would bring about the disappearance. We discuss these results in the context of a crystalline electric field (CEF) ground state.

C1.00288 Multifractal Analysis of the Metal to Insulator Transition in the Three-Dimensional Anderson Model, LOUELLA VASQUEZ, Department of Physics and Centre for Scientific Computing, University of Warwick, CV4 7AL United Kingdom, ALBERTO RODRIGUEZ, Department of Physics and CSC, University of Warwick, CV4 7AL, UK, and Òptico de Física Fundamental, Universidad de Salamanca, 37008 Salamanca, Spain, RUDOLF ROEMER, Department of Physics and Centre for Scientific Computing, University of Warwick, CV4 7AL United Kingdom — The wavefunctions at the metal to insulator transition (MIT) of a disordered system within the Anderson model of localization have been shown to be of multifractal nature. In this paper we use a multifractal analysis to compute for the singularity spectra of very large wavefunctions at the band center. We will show that the singularity spectrum at the MIT is independent of the system size. We compare our results with recent findings and the Wegner prediction.

C1.00289 Superconductivity induced by non-local electron-phonon interaction, KA-MING TAM, University of Waterloo — The effects from commensurate filling, typically in the one-dimensional half-filled systems, often lead to finite charge gap and instability of long wavelength density wave ordering. Various proposals have been suggested recently that some of the one-dimensional electron-phonon coupled systems can be metallic with zero charge gap. However, subsequent studies of these proposals have obtained divergent results. We study an electron-phonon model with non-local electron-phonon interaction, its low energy effective theory unambiguously possess dominant charge gapless superconducting phase at half filling. In this model, the spin-charge coupling at high energy is weakened by the non-local electron-phonon interaction and the charge gap can be destroyed by the suppression of the umklapp process. The existence of the dominant pairing instability in the half-filled system may have an implication on the role plays by the phonon modes in the cuprate superconductor, suggesting that non-local or long range electron-phonon interactions may favor the formation of pairing.

C1.00290 $^1$H NMR Measurements on the Phase Transition of (NH$_4$)$_3$H(SO$_4$)$_2$ Single Crystal, S.H. CHOI, K.S. HAN, S.K. KWON, S.K. NAM, H.H. CHOI, MOOHHEE LEE, Konkuk University, Seoul 143-701 Korea, AE RAN LIM, Jeonju University, Jeonju 560-759, Korea — $^1$H nuclear magnetic resonance (NMR) experiments have been performed in the temperature range of 30 - 300 K at 7 T to investigate the phase-dependent nature of the dynamic network of hydrogen bonds in a (NH$_4$)$_3$H(SO$_4$)$_2$ single crystal. The crystal has six phases, which are ferroelectric, antiferroelectric, incommensurate, antiferroelectric, ferroelastic, and superionic conductor with the respective transition temperatures of 63, 133, 139, 256, and 413 K. The half-filled $^1$H NMR is similar for the ammonium protons and the hydrogen-bonded protons in all range of experimental temperatures. $T_1$ of $^1$H NMR gradually decreases down to 120 K and then starts to steeply increase below 100 K. Then $T_1$ shows an abrupt decrease below 68 K with a sharp minimum at 63 K, where the ferroelectric transition occurs. The $^1$H NMR spectrum shifts to the high frequency side below 63 K due to the ferroelectric phase transition. This temperature dependence of $T_1$ and spectrum confirms a dramatic change in the dynamics of hydrogen bonds associated with the ferroelectric phase transition at 63 K.

C1.00291 Exact thermodynamics of electron hole pairing and ferroelectricity in attractive Hubbard nanoclusters, ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University, GAYANATH FERNANDO, KALUM PALANDAGE, Department of Physics, University of Connecticut, JIM DAVENPORT, Computational Science Center, Brookhaven National — Using analytical diagonalization and symmetries in the small Hubbard clusters, we demonstrate exact mapping between $U > 0$ and $U < 0$ models in the ground state and at finite temperatures for general electron concentration and magnetic fields. We establish equivalency between corresponding phase diagrams for one hole off half-filling at $U > 0$ and in the low spin region for half filled $U < 0$ models. The $U < 0$ model exhibits Fulde-Ferrell-Larkin-Ovchinnikov phase separation into spin-rich and spin-poor analogues to electron pairing for $0 < U < U_C$ [1,2], while at strong coupling regime it provides a mechanism of electron instability with spontaneous (saturated) ferroelectricity, similar to Nagaoka ferromagnetism at $U > U_C$ [1]. The calculated phase diagrams resemble a number of metal dielectric transitions, inhomogeneous paired phases, superconductivity, ferromagnetism and ferroelectricity found recently in transition metal and Nb nanoparticles [3], etc. [3] X. Xu et al., Phys. Rev. Lett. 93, 086803 (2004).
C1.00292 Reversible pressure-induced phase change in eutectic GeSb, DMITRY SHAKHVOROSTOV, University of Western Ontario, London, Ontario, Canada, LIA KRUSIN-ÉLBAM, GLENN J. MARTYNA, DENNIS M. NEWNS, CYRIL CABRAL, JR., IBM T.J. Watson Research Center, Yorktown Heights, NY, USA, SIMONE RAOUX, IBM Almaden Research Center, Almaden, CA, USA, ZAK E. HUGHES, MARTIN H. MÜSER, YANG SONG, University of Western Ontario, London, Ontario, Canada — In phase-change materials (PCMs), typically Ge-Te-Sb based glassy semiconductors, a reversible transformation between a highly resistive (amorphous) and a highly conductive (crystalline) phase is accomplished by Joule heating that melt-quenches PCM into the amorphous state, and thermally anneals it back to the crystalline state. Here we report a room-temperature pressure driven reversible phase change in a binary eutectic GeSb system. From structural and Raman spectroscopy studies, we demonstrate abrupt hysteretic amorphous-to-crystalline and intra-crystalline transitions under a compressive load—unique to the Te-free system—that access with pressure the two extreme GeSb states previously obtained by thermal programming. Using ab-initio molecular dynamics simulations we show that the reverse process occurs under a tensile load. The role of the Peierls gap and Anderson localization in the pressure induced phase change accompanying a metal-insulator transition will be discussed.

C1.00293 Micron-Scale Observation of Nucleating Water Vapor Bubbles, SCOTT PARKER, SUNG CHUL BAE, CHANG-KI MIN, DAVID CAHILL, STEVE GRANICK, University of Illinois at Urbana-Champaign — Surface plasmon microscopy is used to detect nucleation and lift-off of vapor bubbles. Vapor bubbles are generated under pool boiling conditions by heating with a focused Ti-Sapphire laser in the near-infrared region. These bubbles modulate the local index of refraction, thereby altering the local excitation of the surface plasmon which are excited in the Kretschmann geometry and observed with a CCD camera. Altering the surface roughness, we observe how bubbles interact in their earliest stages.

C1.00294 The condensation phenomena of conserve-mass aggregation model with mass-dependent fragmentation, DONG-JIN LEE, SUNGCHUL KWON, YUP KIM, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — We study a conserved mass aggregation model with mass-dependent fragmentation in regular lattice and scale-free networks. In the model, the whole mass m of a site isotropically diffuse with unit rate. With rate $\omega$, a mass $m^k$ is fragmented from the site and moves to a randomly selected nearest neighbor site. Since the fragmented mass is smaller than the whole mass $m$ of a site for $\omega > 1$, the on-site attractive interaction exists for the case. For $\omega = 1$, the model is known to undergo the condensation phase transitions as the density of total masses ($\rho$) increases beyond a critical density $\rho_c$. For $0 < \lambda < 1$, we numerically confirm for several values of $\lambda$ that $\rho_c$ diverges with the system size $L$. Hence in thermodynamic limit, the condensed phase disappears and no transitions take place in one dimension. We also explain that there are no transitions in any dimension. On scale-free networks with degree distribution $P(k) \sim k^{-\gamma}$, we numerically confirm for $\gamma > 3$ that the condensation transitions occurs at $\rho_c > 0$ and its nature is the same as that in regular lattice. However, for $\gamma \leq 3$, the condensation always takes place for $\lambda < \lambda_c$, and masses distribute uniformly without aggregation for $\lambda \geq \lambda_c$. We derive $\lambda_c = 1/\gamma - 1$ via mean-field argument.

C1.00295 Universal and nonuniversal supercritical adsorption in pores, HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA, S.M. GATICA, Department of Physics and Astronomy, Howard University, Washington, D.C., A.D. LUEKING, Department of Energy and Mineral Engineering, The Pennsylvania State University, University Park, PA, J.K. JOHNSON, Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, M.W. COLE, Department of Physics, The Pennsylvania State University, University Park, PA — A recent study of gas adsorption in porous carbons found a common trend in the gas uptake as a function of reduced pressure at the same relative supercritical temperature, with the exception of hydrogen [1]. Using analytical expressions (Henry’s law) and computer simulations (quantum and classical) we demonstrate that the “universal” behavior of the classical gases and the “deviant” behavior of hydrogen can both be understood from simple combining rules and the role of quantum effects. Thus, we reject a hypothetical explanation of the data in terms of small pores permitting just hydrogen to permeate.

C1.00296 ABSTRACT WITHDRAWN

C1.00297 Observation of field-induced magnetic disorder state in one-dimensional antiferromagnet BaCo$_2$V$_2$O$_8$ from NMR, C.S. LUE, C.N. KUO, T.H. SU, ZHANGZHEN HE, MITSURU ITOH, DEPARTMENT OF PHYSICS, NATIONAL CHENG KUNG UNIVERSITY, TAINAN 70101, TAIWAN TEAM, INSTITUTE FOR SOLID STATE PHYSICS, UNIVERSITY OF TOKYO, KASHIWA 277-8581, JAPAN COLLABORATION, MATERIALS AND STRUCTURES LABORATORY, TOKYO INSTITUTE OF TECHNOLOGY, 4259 NAGATSUTA, MIDORI, YOKOHAMA COLLABORATION — We report the results of a $^{51}$V nuclear magnetic resonance (NMR) study on the single crystal BaCo$_2$V$_2$O$_8$ at temperatures between 3k and 300k. This material has been a subject of current interest due to indications of the field-driven magnetic order-disorder transition above 4T. For the present NMR study, we found no abrupt changes in the NMR shift and line width at low temperature as a constant field 7.06T was applied along the $c$-axis, indicative of the absence of magnetic long-range ordering under this field. Hence, the NMR results establish unequivocally the field-induced magnetic disorder state in BaCo$_2$V$_2$O$_8$.

C1.00298 Reentrant Morin Transition in Natural Haematite Crystal at Low Temperature, SEONG-JOO LEE, HYUNOK JUNG, SOONCHIL LEE, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea, JOONGHOE DHO, Department of Physics, Kyungpook National University, Daegu 702-701, Korea — We investigate the magnetic properties of natural haematite ($\alpha$-Fe$_2$O$_3$) crystal at low temperature using a SQUID and $^{57}$Fe nuclear magnetic resonance (NMR). The $M(T)$ curve shows that the net magnetization in the (111) plane vanishes at Morin transition occurring around 260 K but reappears as temperature decreases below 30 K. The $M(H)$ curve shows that the hysteresis exists in the (111) plane and the spin-flop transition also occurs when strong external field is applied in parallel with the [111] direction at low temperature. We obtain the NMR spectra in external magnetic field of up to 7 T at 4.2 K. Comparison of the $M(H)$ curve and the field dependence of the NMR resonance frequency suggests that the antiferromagnetic and the weak-ferromagnetic phases coexist at low temperature. Assuming that the weak-ferromagnetic state at low temperature is the same with that above Morin transition, the amount of the weak-ferromagnetic phase in the antiferromagnetic bath at low temperature is about 3%.

1 We are grateful for the support from the National Science Council of Taiwan. The work done in Japan is support by the Rotary Yoneyama Memorial Foundation.
C1.00299 New Phase transitions in ceramic SrSnO3: Raman scattering and differential thermal analysis, MANOJ SINGH, N.K. KARAN, RAM S. KATIYAR, Department of Physics, University of Puerto Rico, PR, USA, J.F. SCOTT, Department of Earth science, University of Cambridge, UK, H.M. JANG, Department of Materials Science and Engineering Pohang University of Science and Technology, Pohang, Korea, J. F. SCOTT COLLABORATION, H. M. JANG COLLABORATION, R. S. KATIYAR TEAM — We report a continuous or nearly continuous order-disorder transition from orthorhombic (pseudo-tetragonal) to orthorhombic on heating in SrSnO3 at 377 °C. The transition at 377 °C is manifested in an order of magnitude increase in Raman linewidths and in a λ-shaped anomaly in the specific heat. Previous work [Mountstevens et al., Phys. Rev. B71, 220102R (2005)] has interpreted the Pnma – Imma transition at ca. 636 °C as a continuous order-disorder transition and emphasized that this would be unique for an octahedron-tilting transition in oxide perovskite, which are always displacive. Our work on Raman scattering and Differential Thermal Analysis shows that the disorder sets in at much lower temperatures 377 °C, so that the 636 °C transition is disorder-disorder, or a dispersive transition within an already highly-disordered lattice. Hence it may not be as unusual as had been claimed.

C1.00300 11B NMR Study of Spin Structure and Dynamics in TbB4 Single Crystal, S.K. KWON, B.J. MEAN, S.K. NAM, S.H. CHOI, H.H. CHOI, MOOHEE LEE, Konkuk University, Seoul 143-701 Korea, B.K. CHO, GIST, Gwangju 500-712, Korea — 11B NMR measurements have been performed on the single crystal of TbB4 to investigate 4f/3spin structure and dynamics. 11B NMR spectrum, shift, 1/T1 and 1/T2 are measured down to 5 K at 8 T perpendicular to the (110) plane. 11B NMR shift and linewidth are huge and strongly temperature-dependent due to the 4f moments of Tb. In addition, both are proportional to the magnetic susceptibility, indicating that the hyperfine field at the boron site originates from the 4f spins of Tb. Below TN = 43 K, the single broad resonance peak of 11B NMR splits into several peaks reflecting the onset of internal magnetic fields due to the antiferromagnetic spin arrangements. The 11B NMR spectrum at 5 K are generally consistent with the calculation confirming that the collinear spin arrangement is correct. The longitudinal and the transverse relaxation rates, 1/T1 and 1/T2, are independent of temperature above TN and then decreases tremendously indicating the huge suppression of spin fluctuations below TN.

C1.00301 11B NMR Study of Spin Structures and Dynamics in GdB4 Single Crystal, S.K. NAM, B.J. MEAN, S.K. KWON, S.H. CHOI, H.H. CHOI, MOOHEE LEE, Konkuk University, Seoul 143-701 Korea, B.K. CHO, GIST, Gwangju 500-712, Korea — We have performed 11B NMR measurements on a single crystal of GdB4 to investigate 4f/3spin structures and dynamics. 11B NMR spectrum, shift, 1/T1 and 1/T2 are measured down to 5 K at 8 T perpendicular to the c-axis. 11B NMR shift and linewidth are huge and strongly temperature-dependent due to the 4f moments of Gd. In addition, both are proportional to the magnetic susceptibility, indicating that the hyperfine field at the boron site originates from the 4f spins of Gd. Below TN = 42 K, the single broad resonance peak of 11B NMR splits into several peaks reflecting the onset of internal magnetic fields due to the antiferromagnetic spin arrangements. Assuming that the 4f moments of are aligned noncollinearly along the <110> direction in the basal plane perpendicular to the c-axis, we have calculated dipolar fields at the 16 boron nuclear sites from the 4f spins of Tb. The results show that the various peaks of 11B NMR spectrum at 5 K are generally consistent with the calculation confirming that the collinear spin arrangement is correct. The relaxation rates, 1/T1 and 1/T2, are independent of temperature above TN and then decreases tremendously indicating the huge suppression of spin fluctuations below TN.

C1.00302 ABSTRACT HAS BEEN MOVED TO SESSION B33

C1.00303 Atomic Adsorptions on the (020) Surface of α-Pu: A Density Functional Study1, RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — Adsorptions of atomic carbon, nitrogen, and oxygen on the (020) surface of α-Pu have been investigated using the full-potential linearized augmented plane wave plus local basis method. The surface was modeled by a 4-layer periodic slab consisting of a total of 32 Pu atoms. Adsorption energies have been optimized with respect to the distance of the atom from the Pu surface for four adsorption sites, namely the one-fold top, one-fold hollow, two-fold short bridge, and the two-fold long bridge sites. The short bridge site was the most stable adsorption site for C with chemisorption energy of 6.03eV. The long bridge site was the most stable adsorption site for N and O with chemisorption energies of 6.067 eV and 7.32 eV respectively. The work function and net spin magnetic moments respectively increased and decreased in all cases upon chemisorption compared to the bare surface. The density of states and change charge density have been used to analyze the adsorbate-induced changes in the surface electronic structure.

1This work is supported by the U. S. Department of Energy and the Welch Foundation.

C1.00304 Valence Instability and Mass Enhancement in an Extended Periodic Anderson Model, TAKASHI SUGIBAYASHI, YASUHIRO SAIGA, DAI HIRASHIMA, Nagoya University — In CeCu2Si2, CeCu2Ge2 and CeRh1−xIrxIn2, the shape of the superconducting region is asymmetric and the superconducting transition temperature TC reaches its maximum far away from the antiferromagnetic quantum critical point. Onishi and Miyake ascribed the asymmetric behavior of TC to the enhanced valence fluctuations. They introduced the repulsive interaction Ueff between a conduction electron and an f electron, in addition to the Coulomb interaction Uf between f electrons and studied the periodic Anderson model (PAM) with both U and Uf (which is the so-called extended PAM). We investigated the valence instability in the extended PAM and two-fold degenerate extended PAM with the dynamical mean field theory. In these models, we found that the valence instability is observed when Uf is larger than the conduction band width 2V and the f-electron level Ef is deeper than the lower bound of the conduction band, −W. It is also found that the orbital degeneracy suppresses the valence instability. In the parameter region of inducing the valence instability, we investigate the mass enhancement factor Zf which is related to the specific heat.

C1.00305 Experimental Evidence of Fermi-Luttinger Liquid State,1, PHILIPPE DEBRAY, MUSTAFA MUHAMMAD, University of Cincinnati, Cincinnati, OH 45221, STEVEN HERBERT, Xavier University, Cincinnati, OH 45207, RICHARD NEWROCK, University of Cincinnati, Cincinnati, OH 45221 — We have measured Coulomb drag between spatially separated parallel quantum wires, made on AlGaAs/GaAs heterostructures by the split-gate technique, in the absence of tunneling to experimentally probe drag by small forward momentum transfer. Drag between wires of lengths 500 and 300 nm was measured in the one-dimensional transport regime at temperatures in the range 30 mK – 1.2 K. We have observed both positive and negative drag. The temperature dependence of drag of both types is in excellent agreement with that predicted by the recently proposed Fermi-Luttinger liquid (FLL) theory that takes into account the curvature in the fermionic dispersion. Positive drag occurs when the curvature is positive, while negative drag occurs when it is negative.

1This work is supported by the National Science Foundation under grant DMR-0244489.
C.00306 Low Temperature Differential Conductance in Al/AlOx/Sc Tunnel Junctions, SHENG-SHIUAN YEH, JUHN-JONG LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan — We have fabricated several Al/AlOx/Sc tunnel junctions and measured the differential conductances $G \equiv dI/dV$ at low temperatures. Our objective is to study the effect of the coupling between tunneling electrons and localized magnetic impurities (which sit in the insulating barrier) on $G(V,T)$. We observed a crossover from the weak coupling regime to the strong coupling regime. We found that, in both regimes, the $dI/dV$ spectra could be well described by the Appelbaum’s $s$-$d$ exchange interaction theory, with a Kondo temperature $T_{K}^{\text{Appelbaum}} \approx 3.4$ K. On the other hand, we measured zero-bias conductances could be well described by a scaling form predicted by the NRG calculations and a $T_{K}^{\text{NRG}} \approx 38$ K was deduced, being close in agreement with the value of $T_{K}^{\text{Appelbaum}}$. A magnetic field of 4 T was applied at 2.5 K, but no Zeeman splitting in the $dI/dV$ spectra was observed. This absence of Zeeman splitting resulted as a consequence of the high $T_{1}^{\text{K}}$ value found in our junctions.

C.00307 Large drop in dielectric constant at ferrimagnetic ordering of CoCr$_2$O$_4$ thin film as observed by terahertz time domain spectroscopy$^1$, K.R. MAVANI, M. NAGAI, M. SHIRAI, K. TANAKA, Dept. of Physics, Kyoto University, D.S. RANA, I. KAWAYAMA, M. TONOUCHI, Inst. of Laser Engr., Osaka University — Multiferroic spinel CoCr$_2$O$_4$ shows ferrimagnetic transition at $\sim$95 K and, at low temperatures, it shows development of magnetic spin spirals simultaneous to a ferroelectric transition. We have deposited epitaxial CoCr$_2$O$_4$ thin film on MgO(100)substrate and studied the film using temperature dependent terahertz (THz) time-domain spectroscopy. There is a large drop in the dielectric constant ($\varepsilon_1$) to nearly half of its initial value at ferrimagnetic transition of CoCr$_2$O$_4$ thin films in the THz frequency range. This is contrary to few earlier studies by capacitance measurements which showed no significant change in the dielectric constant ($\varepsilon_1$) at ferrimagnetic transition [1]. At lower temperatures, two dielectric anomalies were observed in the temperature dependent $\varepsilon_1$, which correspond to the onset of short-range magnetic spin spirals ($\sim$50 K) and the long-range ordering of the spirals at lower temperature ($\sim$26 K). Our results indicate a magnetoelectric effect at the ferrimagnetic transition of CoCr$_2$O$_4$ thin film in THz frequency range. [1] G. Lawes et al., Phys. Rev. B 74, 24413 (2006).

$^1$This work is supported by JSPS through ‘Grant-in-Aid for Creative Scientific Research’ and ‘Grant-in-Aid for Young Scientists (Start-up)’.

C.00308 Consequences of magnetoelectric interactions on ferroelectric domain structures, P. MAHANANDIA, A.S. TATARENKO, G. SRINIVASAN, Oakland University, Rochester, MI — The standard lift mode of electrostatic force microscopy (EFM) has been utilized to study the influence of magnetoelectric (ME) effect on ferroelectric domain structures in a YIG-PZT bilayer. A PZT disk of thickness=$250 \mu m$ was bonded on to a (111) single crystal YIG on GGG substrates. Randomly oriented domains of PZT are observed in the absence of a dc magnetic filed H. The domains are transformed into a columnar structure when H> 120 Oe is applied to the bilayer. The H-induced changes are mediated by mechanical forces; when a magnetic field is applied to the layered composite, the magnetostriction exerts a stress on PZT, resulting in an induced electric polarization and changes in the domain structure.

C.00309 MIS and MFIS Devices: DyScO$_3$ as a gate-oxide and buffer-layer, R. MELGAREJO, N.K. KARAN, J. SAAVEDRA-ARIAS, D.K. PRADHAN, R. THOMAS, R.S. KATIYAR, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, P O Box 23343, PR 00931 — Metal-Ferroelectric-Insulator-Semiconductor (MFIS) structure is of importance in nonvolatile memories, as insulating buffer layer that prevents interdiffusion between the ferroelectric (FE) and the Si substrate. However, insulating layer has some disadvantages viz. generation of depolarization field in FE film and increase of operation voltage. To overcome this, it is important to find a FE with low $\varepsilon_r$ (compared to normal FE) and an insulating buffer layer with high $\varepsilon_r$ (compared to $\varepsilon_r$ = 3.9 of SiO$_2$). High-k materials viz. LaAlO$_3$, SiN, HfO$_2$, HfAlO etc. have been studied as buffer layers in the MFIS structures and as gate-oxide in metal-insulator-silicon (MIS). Recently, a novel gate dielectric material, DyScO$_3$ was considered and studies indicate that crystallization temperature significantly increased and the film on Si remained amorphous even at 1000 °C annealing. Considering the requirements on crystallization temperature, $\varepsilon_r$, electrical stability for high-k buffer layers, DyScO$_3$ seems to be very promising for future MISFET device applications. Therefore, the evaluations of MOCDV grown DyScO$_3$ as gate-oxide for MIS and the buffer layers for Bi$_{22}La$_{0.75}Ti$_{12}$O$_{30}$ based MFIS structures are presented.

C.00310 Magnetodielectric Effects and Transport Study in LuFe$_2$O$_4$ Single Crystal, TAE HWAN JANG, SANG YOUNG PARK, eSSC & Dept. of Physics, POSTECH, Korea, HAI JOON LEE, SUN HEE KANG, Dept. of Physics, Ulsan Univ., Korea, TAE YEONG KOO, PAL, POSTECH, Korea, SONG BAEK KIM, I-PEM & Dept. of Physics, POSTECH, Korea, ILL WON KIM, Dept. of Physics, Ulsan Univ., Korea, YOON HEE JEONG, eSSC & Dept. of Physics, POSTECH, Korea, SANG WOOK CHEONG, R-CEM and Dept. of Physics & Astronomy, Rutgers Univ., USA — Magnetic, dielectric, and magnetodielectric properties of geometrically frustrated mixed valance LuFe$_2$O$_4$ single crystal are discussed to clarify the charge order, magnetic long range ordering of the spirals at lower temperature ($\sim$26 K). Our results indicate a magnetoelectric effect at the ferrimagnetic transition temperature $T_{M} \sim$100 K in both magnetization and dielectric constant versus temperature curve below the ferrimagnetic transition temperature $T_{M} \sim$225 K has been observed. The sign of magnetodielectric effect (MDE) also changes from positive $T_{N} <$ 26 K to negative $T_{N} < T_{M}$. No field hysteresis in positive MDE temperature region was found. However a large hysteretic behavior in negative MDE below $T_{M}$ with the same magnetic coercive field measured in M (H) curve was observed. This indicates a strong coupling between magnetism and ferroelectricity in the charge and spin frustrated ferrimagnetic LuFe$_2$O$_4$ system.

C.00311 Effect of epitaxial strain on magnetization and photo-control of spontaneous polarization in BiFeO$_3$ films on (LaAlO$_3$)$_{0.3}$Sr$_{0.7}$AlTaO$_{3}$ substrate, D.S. RANA, I. KAWAYAMA, H. MURAKAMI, M. TONOUCHI, Institute of Laser Engineering, Osaka University, Japan — Recent researches on thin films of BiFeO$_3$ have been driven by the need to obtain better multiferric properties by either inducing epitaxial strain or fabrication of magnetoelectric superlattices. The BFO (100) thin films on (LaAlO$_3$)$_{0.3}$Sr$_{0.7}$AlTaO$_{3}$ (100) substrate are highly strained with different physical properties than that of bulk [1]. Given the dependence of ferroelectric polarization of BFO on crystallographic directions, epitaxial thin films $\sim$70nm and 180nm - of BFO were deposited on LSAT (110) substrate. Structure and surface morphology of BFO/LSAT(110) films show that the films with thickness < 80 nm possess a strong in-plane strain while thicker films (150-200nm) are partially relaxed with a bulklike structure. Though the magnetic properties of BFO/LSAT(110) films are nearly independent of structure, the spontaneous polarization and the ferroelectric properties (probed by terahertz emission) are strong characteristic of structure. These results emphasize the importance of epitaxial strain induced tailoring of the ferroelectric properties of BiFeO$_3$ film along (110) crystallographic direction. 1. D.S. Rana et al, Phys. Rev. B 75, 060405 (2007).

C.00312 Anomalies in the thermoelectric power in cuprates from strong electron correlation, SHILADITYA CHAKRABORTY, DIMITRIOS GALANAKIS, PHILIP PHILLIPS, University of Illinois at Urbana- Champaign — The thermoelectric power data in hole-doped cuprates show a sign change on increasing the hole doping from the underdoped to the overdoped regime. The origin of this anomaly is debatable, and there exist multiple explanations for it. Phonon drag is one of the more widely accepted explanations. Our approach, instead, is to investigate the behavoir of the thermoelectric power from a purely electronic perspective. We employ Cluster Dynamical Mean Field Theory (CDMFT) on a four site square plaquette to study the thermoelectric power in the 2-d Hubbard model as a function of hole doping, temperature and $U/t$ ratio. We observe a sign change in the thermoelectric power in qualitative agreement with experimental data. The sign change vanishes for small values of $U/t$, suggesting that strong electron correlations are responsible for this phenomenon.
C1.00315 Rectification effects in InAs/AlGaSb three-terminal ballistic junctions, MASATOSHI KOYAMA, Nanomaterials Microdevices Research Center, Osaka Institute of Technology, TATSUYA INOUE, NAOKI AMANO, TOSHIHIKO MAEMOTO, SHIGEHIKO SASA, MASATAKA INOUE, NANOMATERIALS MICRODEVICES RESEARCH CENTER, OSAKA INSTITUTE OF TECHNOLOGY TEAM — We report on the fabrication and the DC characterization of InAs/AlGaSb three-terminal ballistic junctions consisting of three quantum-wire T-shaped structures. InAs/AlGaSb quantum wells were grown by molecular beam epitaxy, and the three-terminal ballistic junctions were defined using electron beam lithography. Typical electron mobility of 80,000 – 200,000 cm²/Vs and sheet carrier density of 1.0 – 2.0 x 10¹² cm⁻² were observed at 77K. Ballistic electron transport properties are due to the one-dimensional (1D) nature of electrons in InAs and dramatic changes in scattering probability from the 2D electron system, which are expected to occur at higher temperatures. We measured the rectified output voltage, Vᵣ at the central branch of the devices at various temperatures. Nonlinearity and negative voltages at the central branch, regardless the polarities of the source-drain (left and right branch) voltage, were observed at each temperature. Clear rectification effects were observed in the ballistic junctions even at room temperature. Details of the triode characteristics in the InAs/AlGaSb ballistic devices will be discussed at the conference.

C1.00316 MnScN(001)/MgO(001) films grown by molecular beam epitaxy: a possible dilute magnetic semiconductor, ARTHUR R. SMITH, Ohio University, COSTEL CONSTANTIN, Seton Hall University, UTKUR MIRSAIDOV, University of Illinois at Urbana Champagne, JOHN MARKERT, University of Texas at Austin — Considerable interest has been of late in finding a room temperature dilute magnetic semiconductor. Recently, theoretical calculations had predicted Curie temperature to be above 400 K for the films with 3% Mn concentration into the MnₓSc₁₋ₓN system. In this study, MnₓSc₁₋ₓN films (with x = 3-5%) were grown on ScN(001)/MgO(001) substrates by radio frequency plasma assisted molecular beam epitaxy. The buffer layer of ScN(001) was grown on top of MgO(001) at Tₑ ≈ 800 °C and with a thickness of ~50 nm. The MnScN film was grown at Tₑ ~ 520 °C and with a thickness of ~290 nm. Post-growth x-ray diffraction measurements show that MnₓSc₁₋ₓN alloys follow the Vegard’s law. The hysteresis magnetic data measured with the superconducting quantum interference device show possible ferromagnetic behavior for the MnₓSc₁₋ₓN films with a Curie temperature of ~50 K, but additional data is needed to establish the conclusiveness of the results. Work supported by NSF.


C1.00317 Characterization of p-InGaAsSb/n-GaSb and p-GaAs/n-GaAs Structures for the Fabrication of Fusion-Stacked Solar Cells, M.L. GOMEZ-HERRERA, J.L. HERRERA-PEREZ, CICATA-IPN, U. Legaria, P. RODRIGUEZ-FRAGOSO, J.G. MENDOZA-ALVAREZ, Physics Dept. Cinvestav-IPN, I. RIECH, Fac.Ing.Fisica. UAdEY, G. TORRES-DELGADO, U.Queereto. Cinvestav-IPN — We are developing a two-stacked solar cell, using for the infrared portion a p-InGaAsSb/n-GaSb heterostructure, and a p-GaAs/n-GaAs for the visible part. Both structures were grown using the liquid phase epitaxy growth technique, and doping at different levels the p-type layers in order to obtain p-n junctions with different electrical characteristics and depletion layer depths. We present results on the characterization of both structures using the photoluminescence spectroscopy to characterize the layer crystalline quality, and the photoacoustic effect to characterize the layer-substrate interface for both structures. Also, we present the results on the I-V characterization and spectral response of both p-n structures for the different doping levels in the p-type layers used. Finally, details on the fusion process to stack the two solar cells are discussed.

We acknowledge financial support from Conacyt-Mexico.

C1.00318 Optical Properties of GaNₓAs₁₋ₓ Thin Films Grown on Si Substrates by r f. Sputtering, J.G. MENDOZA-ALVAREZ, O. ZELAYA-ANGEI, A. CRUZ-OREA, Physics Dept. Cinvestav-IPN, J.S. ARIAS-CERON, CICATA-IPN. U. Legaria, J.A. CARDOÑA-BEDOYA, Depto. Fisica. U. del Tolima — GaNₓAs₁₋ₓ ternary alloys in the GaN-rich side, are expected theoretically to have band-gap energies in the full range of the visible spectrum for just a small change in the nitrogen concentration in the range of about 70-85%. Using the r. f. sputtering and the laser ablation film deposition techniques, we have reported the growth of ternary GaNAs layers with band-gap energies in the range between 1.4 to 2.6 eV. In this work we report the growth of GaNAs thin films on Si substrates using the r. f. sputtering technique at high substrate temperatures; the r. f. power was varied in order to control the nitrogen incorporation in the films. The low temperature photoluminescence (PL) and the photoacoustic (PA) spectroscopies were used to characterize the optical properties of the series of GaNₓAs₁₋ₓ As films grown with different stoichiometries. We discuss the origin of the transitions observed in the PL spectra and the shoulders around 2.5 eV observed in the PA spectra.

We acknowledge financial support from Conacyt-Mexico.

C1.00319 Differential Magnetoresistance Oscillations induced by Microwave and DC Electric Fields, MAXIM KHODAS, University of Minnesota, MAXIM VAVILOV, University of Wisconsin Madison — We study magnetoresistance oscillations in two-dimensional electron systems induced by AC and DC fields. We find the position of the maxima and minima in the differential magnetoresistance, r(εₓ,kₓ) and evaluate the amplitude of magneto-oscillations in terms of various microscopic parameters of the system. We compare our findings with the results of recent experiments by W. Zhang, Phys. Rev. Lett. 98, 106804 (2007).
C1.00320 First-Principles Theory of Ordering, Phase Separation, and Phonon Scattering in Thermoelectric LAST (Lead-Antimony-Silver-Telluride) alloys\(^1\), SERGEY V. BARABASH, VIDVUDS OZOLINS, UCLA, CHRIS WOLVERTON, Northwestern University — Bulk LAST (Pb\(_{1-x-y}\)Ag\(_x\)Sb\(_y\)Te\(_2\)) alloys exhibit high thermoelectric figure of merit (ZT \(\sim\) 2 at 800K, considerably exceeding ZT of pure PbTe or AgSbTe\(_2\), and nano-scale inhomogeneities, origin of which is poorly understood. The atomic structure of the nano-regions, as well as that of the pure AgSbTe\(_2\), remains the subject of an experimental debate. Using density-functional theory (DFT), we calculate the composition-temperature phase diagram and vibrational spectra of Pb\(_{2-x-y}\)Ag\(_x\)Sb\(_y\)Te\(_2\) alloys. We predict that the experimentally observed nanoscale inhomogeneities are due to the precipitation of ordered AgSbTe\(_2\) phases. Two types of cation order type closely compete in AgSbTe\(_2\), the dominant order type being D4; the predicted hypothetical order-disorder transition temperature exceeds the melting temperature of pure AgSbTe\(_2\). The miscibility gap between solid PbTe and AgSbTe\(_2\) phases is highly asymmetric, with a high solubility of PbTe in ordered AgSbTe\(_2\). We also characterize the shape of coherent precipitates. Finally, the phonon spectra of AgSbTe\(_2\) and PbTe suggest that boundary scattering of acoustic phonons causes the observed suppression of thermal conductivity.


C1.00321 Oxygen adsorption on Cu/ZnO (0001) – Zn. \(^{1}\)PATRICIO HÄBERLE, UTFSM, Valparaiso, MATTHIAS BATZILL, Univ. of South Florida, ULRIKE DIEBOLD, Tulane Univ., PAOLA LAZCANO, UTFSM, Valparaiso — By using plasma assisted deposition we have adsorbed oxygen onto the Cu/ZnO(0001)-Zn surface. Cu was deposited on the sputtered-annealed ZnO substrate at room temperature, which was later exposed to oxygen. Using X-ray photoelectron spectroscopy (XPS) we verified the effect of the oxidation procedures on the electronic structure of the interface. Our results are consistent with a partially oxidized Cu layer, in which CuO is mainly located at the interface between ZnO and the adsorbed Cu islands. Further Cu deposition induces the formation Cu2O. Annealing the sample in UHV induces further oxide reduction. The oxidation is reversible and metallic Cu is recovered on the top layer.

C1.00322 Nucleation and stochiometry dependence of rutile-TiO\(_2\) thin films grown by plasma-assisted molecular beam epitaxy. COSTEL CONSTANTIN, Seton Hall University, KAI SUN, University of Michigan, R.M. FEENSTRA, Carnegie Mellon University — Considerable interest has been shown of late in transition-metal oxides. One case is the titanium dioxide system, which can have a high degree of disorder, as compared to the samples prepared WITH the pseudo 1 × 1 Ga-rich surface reconstruction, and the other set, WITHOUT the pseudo 1×1. On top of these two type of surfaces, the rutile-TiO\(_2\) thin films were grown at T\(_s\) \(\sim\) 600 \(^\circ\)C, and with a thickness \(\sim\) 40 – 50 nm. During growth, reflection high-energy electron diffraction indicated a reversible stochiometry transition from O-rich to Ti-rich growth. Post-growth x-ray diffraction measurements performed on the samples WITHOUT the GaN pseudo 1×1, show the presence of additional peaks at 2\(θ\) \(=\) 52.9\(^°\), which implies the existence of additional phases. In addition, the high-resolution transmission electron microscopy performed on these samples show a high degree of disorder, as compared to the samples prepared WITH the pseudo 1×1. Work supported by ONR.

\(^{1}\)Z. J. Luo et al., Appl. Phys. Lett. 79, 2803

C1.00323 Study of the crystalline structures of the syndiotactic polystyrene (sPS) under mechanical deformation. SUGURU NAGASAKA, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University, Japan — Polystyrene (PS) has become one of the important, yet complicated semi-crystalline materials since the successful synthesis of the syndiotactic PS (sPS) by Ziegler-Natta catalyst. Since then, sPS has been actively investigated and four different crystalline forms (\(α\), \(β\), \(γ\) and \(δ\)), two mesomorphic forms and various clathrate forms have been found, indicating complex feature of its crystalline structures. Among the four crystalline forms, \(α\) and \(β\)-crystals can be obtained by different annealing processes and both crystalline structures comprise the same all-trans planar conformation. In this work, \(β\)-crystal structure was made by high temperature annealing and the sPS with \(β\)-crystal structure was mechanically stretched above the glass transition temperature of sPS, followed by the crystalline transition analysis studied by FT-IR.

C1.00324 Magnetic Field Effects on Intersystem Crossing in Polaron-Pair, Excitonic, and Charge-Transfer States in Organic Semiconducting Materials\(^1\), LIANG YAN, BIN HU, University of Tennessee — The singlet-triplet intersystem crossing can be magnetic field dependent in organic semiconductor molecules. This field-dependent intersystem crossing accounts for the magnetic properties of these non magnetic organic semiconductor molecules. Therefore, the study of the dependence of magnetic field on the intersystem crossing can enhance the understanding of intrinsic magnetic responses of excited states and also exped the application of non magnetic organic materials to magnetic devices. In this report we will present our recent investigations: magnetic field effects on singlet-triplet intersystem crossing based on the selected polaron-pair, excitonic, and charge-transfer excited states by using magnetic field-dependent electroluminescence, photoluminescence, and photocurrent. Our experimental results show that the intersystem-crossing dependence of magnetic field significantly decreases as the internal electron-hole distance is reduced in an excited state. This phenomenon indicates that the electron-hole distance essentially determines the intersystem-crossing dependence of magnetic field through the competition between the Zeeman splitting of triplet sublevels caused by applied magnetic field and the intrinsic singlet-triplet energy difference generated by the distance-dependent spin-exchange interaction. As a result, changing the electron-hole distance presents a new mechanism to magnetically tune the optoelectronic properties of non magnetic organic semiconductor molecules.

\(^{1}\)The research is supported by AFOSR and NSF

C1.00325 Using genetic algorithms to search for an optimal portfolio strategy and test market efficiency , HAOWEN XI, EDWARD MANDERE, Bowling Green State University — In this numerical experiment we used genetic algorithms to search for an optimal portfolio investment strategy. The algorithm involves having a “manager” who divides his capital among various “experts” each of whom has a simple fixed investment strategy. The expert strategies act like population of genes which experiencing selection, mutation and crossover during evolution process. The genetic algorithm was run on actual portfolio with stock data (DowJones 30 stocks). We found that the genetic algorithm overwhelmingly selected optimal strategy that closely resembles a simple buy and hold portfolio, that is, evenly distribute the capital among all stocks. This study shows that market is very efficient, and one possible practical way to gauge market efficiency is to measure the difference between an optimal portfolio return and a simple buy and hold portfolio return.
C1.00326 Magnetic Study of Exciton-Charge Reaction in Organic Phosphorescence-Based Light-Emitting Diodes

MING SHAO, BIN HU, University of Tennessee — The capture of electron and hole leads to the singlet and triplet excitation formation at 1.3 ratio in organic light-emitting diodes (OLEDs) of fluorescent conjugated molecules. This significantly limits the quantum efficiencies of singlet light emission from OLEDs. The alternative option is to use triplet emission from phosphorescent molecules to ultimately increase the quantum efficiencies of OLEDs. In this report we will present our recent studies of triplet excitation-charge reaction in most efficient phosphorescence-based OLEDs by using magnetic field-dependent electroluminescence and excited state-related magnetoresistance. Our experimental results show that the electrically generated excitons can react with charge carriers with two consequences: detrapping charge carriers or splitting electrons and holes in excited states. Nevertheless, the triplet excitation-charge reaction presents a significant challenge to increase the quantum efficiencies of OLEDs towards the theoretical limit of 100%. Furthermore, we observed that the charge-trapping reaction can be adjusted by changing the balancing degree of bipolar electron and hole injection. Therefore, tuning the bipolar injection can form a mechanism to control the triplet-trapping reaction and to consequently improve the quantum efficiencies of phosphorescence-based OLEDs.

1The research is supported by NSF and AFOSR.

C1.00327 Enhanced Photovoltaic Effect from Nanocomposite of Treated PbS Quantum dots and π-conjugated polymers

XIAOMEI JIANG, JIAN ZHANG, University of South Florida — We report novel type of hybrid solar cells based on nanocomposites of conjugated polymers (polythiophene) and IR-sensitive PbS nanocrystals that have a size-tunable energy gap between ca. 0.7 and 1.6 eV. Thin film cells show very good diode characteristics and sizable photovoltaic response. The good performance of our devices in both photovoltaic and photodiode regimes indicates quite efficient charge separation between the polymer and QD components. To further facilitate charge separation and transport in these composite structures, we applied various ligands exchange (pyridine, butylamine and octylamine) to the quantum dots prior to device fabrication. We find noticeable increase of photocurrent due to more efficient charge separation when the original bulky oleic acid ligand of the nanocrystals was replaced by these much smaller ligands. We have conducted mobility measurement of PbS QDs with different sizes, both in pure QD film and the hybrid nanocomposite with polymers. Both electronic and optical device characterizations were carried out. Specifically, we observe indications of a rapid increase in the photocurrent at spectral energies in correlation with the size-dependent energy gap of the QD component.

C1.00328 Studies on the parameters affecting the adhesion between Diamond-Like Carbon (DLC) films and polyolefin substrates

YUUMA NAKAMURA, Department of Mechanical Engineering, Keio University, Japan. TERUMITSU HASEBE, Department of Radiology, Tachikawa Hospital, Japan. AKI KAMURO, Department of Transfusion Medicine, University of Tokyo Hospital, Japan. TETSUYA SUZUKI, ATSUSHI HOUTTA, Department of Mechanical Engineering, Keio University, Japan. Polyolefins coated with thin Diamond-Like Carbon (DLC) films are particularly attractive for effective control of the surface and mechanical properties of the polyolefins and the adhesion between the DLC and the polyolefins determines the major properties: if the adhesion force is not sufficient, DLC film is easily peeled off from the polyolefin substrate, eventually degrading the whole highly-controlled DLC-polyolefin system. In this work, we evaluated the adhesion between DLC films and various polyolefin substrates through T-peel testing using tensile tester. DLC films were deposited on each polyolefin substrate by plasma enhanced chemical vapor deposition (CVD) method using acetylene gas. High-density polyethylene (HDPE), low-density polyethylene (LLDPE), linear-low-density polyethylene (LLDPE), isotactic polypropylene (iPP) and syndiotactic polypropylene (sPP) were introduced as polyolefin materials. It was found that molecular structures and annealing conditions had significant effects on the adhesion between DLC and the polyolefins.

C1.00329 Raman scattering from the CaC$_6$ superconductor

A. MIALITISIN, Rutgers University, J. KIM, R. KREMER, MPI fuer Festkoerperforschung, G. BLUMBERG, Bell Labs, Alcatel-Lucent — A polarized Raman scattering study has been performed on bulk 1st stage intercalated graphite CaC$_6$ crystals at sub-T$_c$ temperatures. We identify all three Raman active E$_g$ bands expected for the R$_m$6 space group of CaC$_6$ at 440, 1120 and 1508 cm$^{-1}$ and find them to be in agreement with zone center modes predicted by first principles calculations of phonon dispersion. In addition the equivalents of the graphite G and D bands are observed at respective frequencies. Inherent to the disorder induced double resonant scattering process the D band shifts from 1308 cm$^{-1}$ to 1332 cm$^{-1}$ upon the change of the excitation laser wavelength from 647 nm to 476 nm. Assuming linear dependence of the D band peak position as a function of excitation energy this translates to the frequency shift of 35 cm$^{-1}$/eV. By comparing the integrated intensity of the G band at 1582 cm$^{-1}$ in CaC$_6$ to the one in kish graphite the relative fraction of higher stage domains to the 1st stage intercalation is estimated to be less than 0.2%. Finally upon the superconducting phase transition we observe a $\Delta$ peak with the frequency of 24 cm$^{-1}$ at 5 K. With temperature increase this peak persists roughly up to the SC phase transition at 11.6 K and shows temperature dependence consistent with the strong coupling regime.

M. Calandra and F. Mauri, PRL 95, 237002 (2005).

C1.00330 Ni-Impurity Effect in High-T$_c$ Cuprates Studied by Neutron Scattering and XAFS Spectroscopy

HIARUHI HIRAKA, SHUICHI WAKIMOTO, MASAKI MATSUDA, DAIJU MATSUMURA, YASUO NISHIHATA, JUN-ICHIRO MIIZUKI, KAZUYOSHI YAMADA, Tohoku University — Neutron scattering experiments using La$_{2-x}$Sr$_x$Cu$_{1-y}$Ni$_y$O$_4$ clarified that the parallel spin-density modulations (SDMs) in the superconducting phase are susceptible to Ni, in the same way as the diagonal SDMs in the insulating spin-glass phase. Ni substitution reduces the mobile hole concentration from x to y. Polarized XAFS measurements using Ni K-edge probe two types of Ni valence states; Ni$^{2+}$ and Ni$^{2+}$+Ni$^{3+}$. It indicates that a strong hole localization occurs around Ni, resulting in an effective spin-1/2 value at Ni sites. Therefore, a charge dopant nature of Ni is most likely realized when x $>$ y.

C1.00331 Spin transfer torque switching in perpendicular magnetic tunnel junctions with Co based multilayer

TOSHIHIKO NAGASE, Corporate R&D Center, Toshiba Corporation, KATSUYA NISHIHATA, MASAHIKO NAKAYAMA, NAOHARU SHIMOMURA, MINORU AMANO, TATSUYA KISHI, HIROAKI YODA — It has been reported that spin transfer torque switching in the perpendicular magnetic device has the advantage of improving the spin-torque efficiency in comparison with the in-plane one [1, 2]. Our previous study was the first time to demonstrate the spin transfer switching in perpendicular magnetic tunnel junctions (MTJs) using TbCoFe alloy. In this paper, we report studies on the spin-torque efficiency in MgO based perpendicular MTJs consisting of CoFeB wedge/Co/PtCo/Co/Pd free layer and FePt/CoFeB reference layer. The damping constant $\alpha$ of the free layer increases in the thinner parts of the CoFeB thickness because of the effect of spin pumping. The ratio of the switching current density to the thermal stability factor (Jc/\Delta), which corresponds to the spin-torque efficiency, was estimated. It was found that the free layer with the thicker CoFeB had a lower Jc/\Delta because of its smaller $\alpha$. Our results experimentally clarify that reducing $\alpha$ leads to achieving the low switching current.


This work was partially supported by NEDO.
C1.00332 Electric Field-Induced Effects on Single-Walled Carbon Nanotube Photoluminescence, ANTON NAUMOV, SERGEI BACIHOLO, R. BRUCE WEISMAN, Rice University, Houston, TX — An investigation of the fluorescence emission of single-walled carbon nanotubes (SWNTs) in electric fields will be described. HiPco SWNTs were embedded in poly(methylmethacrylate) (PMMA) films deposited onto the surface of microscope slides with ITO or interdigitized gold electrodes. The fluorescence of individual semiconducting SWNTs was then observed using a microscope coupled to a near-IR spectrophotograph and an InGaAs 2-D camera. Bulk samples of SWNTs in polymer were studied with a spectrofluorometer. When SWNTs in PMMA were subjected to electric fields of up to $10^7$ V/m, a drastic decrease in fluorescence intensity was observed. This quenching is well described as a single-parameter inverse hyperbolic cosine function of applied field. The quenching effect is also dependent on the angle between SWNT and field, the length of the SWNT, and SWNT diameter (exciton binding energy). The quenching mechanism may involve both exciton dissociation in an electric field and free carrier effects. The latter were suggested by studies of long nanotubes.

C1.00333 Scaling Laws for NanoFET Sensors, QI-HUO WEI, FU-SHAN ZHOU, Liquid Crystal Institute, Kent State University — In this paper, we report our numerical studies of the scaling laws for nanoplate field-effect transistor (FET) sensors by simplifying the nanoplates as random resistor networks. Nanowire/tube FETs are included as the limiting cases where the device width goes small. Computer simulations show that the field effect strength exerted by the bonding molecules has significant impact on the scaling behaviors. When the field effect strength is small, nanoFETs have little size and shape dependence. In contrast, when the field-effect strength becomes stronger, there exists a lower detection threshold for charge accumulation FETs and an upper detection threshold for charge depletion FET sensors. At these thresholds, the nanoFET devices undergo a transition between low and large sensitivities. These thresholds may set the detection limits of nanoFET sensors. We propose to eliminate these detection thresholds by employing devices with very short source-drain distance and large width.

C1.00334 Fabrication and magnetic characterization of ferromagnetic nanotubes, REHANA SHARIF, SHAMAILA SHAHZADI, HAN YUNAN, MING MA, HAN XIU-FENG, Institute of Physics Chinese Academy of Sciences — During the last decade, interesting properties of magnetic nanowires have attracted much attention. Besides their interesting basic properties, there is evidence that these can be used in the fabrication of new nanodevices. Recently, magnetic nanotubes have successfully fibred in graphene and have become a symbol of new and fast developing research area of nanotechnology because of their technological applications in patterned recording media, magnetic sensors and magnetic biotechnology. Ferromagnetic nanotubes have been fabricated using templates (Alumite, PCTE) which can provide us a straight forward route to fabrication of the nanotubes. The anisotropy of the tubes is governed by shape anisotropy and the switching field of the tubes is consistent with that expected from curling mechanism in which the magnetization rotates within the plane of the tube wall.

C1.00335 Possible nano-graphene devices having topology origin edge states, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — In nanometer scale graphene structures, edge-localized surface states may appear in specified edges. Evidences of the edge states has been given by the ultra high vacuum STM/STS observation of well-characterized edges of graphene structures.[1,2] The density functional theory supported both appearance of edge states and existence of localized magnetism in a characterized Hydrogenated graphene structures within the local-spin-density approximation.[3] In this study, we reconsider appearance of the edge states due to network topology of π orbitals of graphene, which is used in designed structures for nano-meter scale graphene-based devices. We consider graphene structures bridging two metallic Ni electrodes. For the Ni (111) surface, epitaxial growth of graphene is possible. We assume that the Ni electrode has a sharp straight edge. The interface between graphene and Ni structure creates a boundary condition for conducting electrons in the graphene, since it is known that a gap is formed in the electronic states of graphene pasted on Ni. The gap is much enhanced by fluorination of graphene on Ni. There are two types of boundary for the graphene structures, which may be classified into zigzag and Klein’s edges. Thus, we can design a graphene-based magnetic FET structure with Ni electrodes by possible partial fluorination of graphene. First-principles electronic structure calculations for this structure is given. [1] Y. Kobayashi, K. Fukui, T. Enoki, K. Kusakabe and Y. Kaburagi, Phys. Rev. B 71, 193406-1-4 (2005). [2] Y. Kobayashi, K. Fukui, T. Enoki and K. Kusakabe, Phys. Rev. B 73, 125415-1-8 (2006). [3] K. Kusakabe and M. Maruyama, Phys. Rev. B 67, 092406-1-4 (2003).

C1.00336 Demixing of Charged Nanoparticle-Polymer Mixtures: A Simulation Study, BEN LU, ALAN R. DENTON, North Dakota State University — The phase behavior of mixtures of charged nanoparticles and neutral polymers is studied by computer simulation. Adapting the classic Asakura-Oosawa-Vrij model, the polymers are modeled as coarse-grained effective spheres that are mutually ideal (theta solvent), but can overlap the nanoparticles with a penetration energy that mimics a loss of chain conformational entropy. Although monodisperse in chain length, the polymers fluctuate in radius of gyration in response to the nanoparticles. Within the primitive model of charged colloids, the nanoparticles are modeled as charged hard spheres, governed by effective electrostatic interactions, including a repulsive screened-Coulomb (Yukawa) pair potential and a one-body volume energy. To investigate demixing behavior, constant-NPT Gibbs ensemble Monte Carlo simulations are performed over ranges of nanoparticle-polymer size ratio, nanoparticle charge, and salt concentration. In the limit of neutral nanoparticles, simulation results are compared with predictions of density-functional theory.

C1.00337 Topological Validation of Morphology Modeling by Reverse Monte Carlo Analysis of Two-dimensional Scattering Patterns, KATSUMI HAGITA, National Defense Academy, JAPAN, TAKASHI TERAMOTO, Chiose Institute of Science and Technology — We presented a new method of morphology modeling using coarse-grained particles from multiple two-dimensional (2D) patterns of structure factors, which can be obtained from small angle x-ray scattering (SAXS). Reverse Monte Carlo (RMC) technique is extended for multiple 2D patterns. It is motivated by SAXS experiments of kinetic pathway from hexagonal perforated lamellar structure to double gyroid (DG) structure in the surfactant/water systems. For the first test, we examine reproducibility of a DG morphology. As a reference configuration, we obtain positions of particles forming DG morphology are generated in a computer using the equation of DGs surface. Inputs of this extended RMC method are calculated from this reference configuration. The configurations obtained from this extended RMC method are examined by the Betti numbers which are mathematical indexes to classify complicated inter-connected three-dimensional structures and are given by Computational homology (Chomp) analysis. Combination of RMC and Chomp is examined as a new and useful approach for connecting scattering experiments to mathematics for 3D morphology.

C1.00338 Thermal Deflection of Nanojets, WEI KANG, UZI LANDMAN, School Of Physics, Georgia Institute of Technology — Generation of fluid jets of reduced sizes, down to the nanoscale [1], is a topic of continuing interest from both basic science and technological perspectives. One of the challenges pertains to the ability to control the direction of propagation of the jet. For macroscopic jets, including those with radii in the several micron range, a common method to vary the propagation direction is through the deflection of charged droplets, or as suggested more recently, via asymmetric heating that affects the surface tension and viscosity of the jet. Here we discuss a jet-bending method based on asymmetric heating of a fluid flowing in a cylindrical nozzle, where the main contribution to the deflection of the emanating nanojet is due to asymmetric evaporation near the exit, which results in a directional thrust that deflects the nanojet. Molecular dynamics simulations demonstrating bending of propane nanojets are discussed. [1] M. Moseler, U. Landman, Science 289, 1165 (2000); W. Kang, U. Landman, Phys. Rev. Lett. 98, 064504 (2007).
C1.00339 Clustering Dynamics of Ultra-fine Particulate Systems, MEENAKSHI DUTT, JAMES ELLIOTT, University of Cambridge — Length scales of particles and their surrounding medium strongly determines the nature of their interactions with one another and their responses to external fields. We are interested in systems of ultrafine particles (0.1 - 1.0 micron) such as volcanic ash, solid aerosols, or fine powders for pharmaceutical inhalation applications. We develop a numerical model for these systems using the Derjaguin-Muller-Toporov (DMT) adhesion theory along with the van der Waals attraction between the particles and their contact mechanical interactions. We study the dynamics of these systems in the absence and presence of gravity by controlling the particle size, and thereby, the surface properties of the particles. The high surface energies of these particles cause them to agglomerate as they gravitationally settle. We explore their internal structure as a function of their particle size.

C1.00340 Qubit Entanglement Driven by Remote Optical Fields, MUHAMMED YONAC, University of Rochester — We examine the entanglement between two qubits, supposed to be remotely located and driven by independent quantized optical fields. No interaction is allowed between the qubits, but their degree of entanglement changes as a function of time. We report a collapse and revival of entanglement that is similar to the collapse and revival of single-atom properties in cavity QED.

C1.00341 Optical Characterization of Biological Tissues, FREDERICK BARRERA, DHIRAJ SARDAR, ANDREW TSIN — University of Texas at San Antonio, San Antonio, Texas 78249. An in-depth characterization of optical properties of biological tissues has been performed. The wavelength-dependent total diffuse reflection ($R_d$) and total transmission ($T_d$) measurements have been taken for individual tissue by using a double-integrating sphere setup. The index of refraction of the tissue will be determined using conventional optical techniques. The Inverse Adding Doubling (IAD) computational method is applied to the measured values of $n$, $R_d$, and $T_d$ to calculate the optical absorption and scattering coefficients as well as the scattering anisotropy coefficients of these tissues. The $R_d$ and $T_d$ determined by the IAD method were compared with those generated by the Monte Carlo simulation technique. A thorough comparison of the scattering characteristics of these tissues has been made. Furthermore, a comparison of these optical scattering and absorption coefficients calculated by IAD method were compared to the values determined by the Kubelka-Munk model.

3:06PM D1.00002 Density-functional theory of superconductivity, E.K.U. GROSS, Freie Universitat Berlin — A prominent challenge of modern condensed-matter theory is to predict reliably material-specific properties of superconductors, such as the critical temperature. The traditional model of Bardeen, Cooper and Schrieffer (SCS) properly describes the universal features that all conventional superconductors have in common, but it is not able to make accurate predictions of material-specific properties. To tackle this problem, a density-functional formalism has been developed [1] which describes superconductors in thermal equilibrium in terms of three quantities: the ordinary density, the superconducting order parameter, and the nuclear N-body density. These three “densities” are determined self-consistently through a set of Kohn-Sham equations. Approximations of the universal exchange-correlation functional are derived on the basis of many-body perturbation theory. In this way, a true ab-initio description is achieved which does not contain any adjustable parameters such as the $\mu^*$ of Eliahouberg theory. Numerical results for the critical temperature, the isotope effect, the gap function and the jump of the specific heat will be presented for simple metals, for MgB$_2$ and CaBeSi, and for calcium intercalated graphite (CaC$_6$) [3]. Furthermore, results for Li, Al, K, and H under pressure will be discussed. The calculations explain why Li and Al behave very differently, leading to a strong enhancement of superconductivity for Li and to a clear suppression for Al with increasing pressure [4]. For K we predict a behavior similar to Li, i.e. a strong increase of $T_c$ with increasing pressure. Finally, hydrogen is found to be a three-gap superconductor whose critical temperature increases with increasing pressure until about 100K (at 500 GPA).

3:42PM D1.00003 Remarks on Molecular Density Functional Theory, ROBERT PARR, University of North Carolina — The dft of finite molecular systems possesses unique special characteristics that produce challenges not yet met and promises not yet realized. I describe several of the problems in this subject with which we have been struggling.

4:18PM D1.00004 The Partition Problem; Insights from Density Functional Theory, MORREL H. COHEN, Rutgers University; Princeton University — How to partition a system into its components, the atoms in molecules problem and its multi-atomic generalizations, arises ubiquitously in physics, chemistry, and materials science. It is central to population analysis, chemical reactivity theory, issues of transferability, and relevant to computational methods for very large systems such as QM-MM and O(N) schemes. At issue is the decomposition of the total electron density into contributions from each part, whence the relevance of density functional theory. My collaborators and I have developed a new, exact scheme, partition theory, for that decomposition. It is based on the Perdew, Parr, Levy, and Baldiz ensemble formulation of density functional theory. In this talk, the elements of partition theory will be described, including its formal structure, a dynamical version for efficient computation, and quantitative illustrations of its central features via the partition of very simple systems.
2:30PM D2.00002 Doping Dependent Anisotropic Electronic Scattering rate in LSCO, JOEL MESOT, ETH Zurich and PSI — An angle-resolved photoemission study of the scattering rate in the normal and superconducting states of the high-temperature superconductor La(2-x)Sr(x)CuO(4) as a function of binding energy and momentum will be presented. We report that, close to optimal doping, the scattering rate scales linearly with binding energy up to a high-energy scale E1. The scattering rate is found to be strongly anisotropic, with a minimum along the nodal direction of the superconducting gap. Since both the degree of anisotropy and the energy dependence of the scattering rate appear to be strongly doping dependent, possible connections to a quantum-critical point will be discussed.

3:06PM D2.00002 Doping Dependent Anisotropic Electronic Scattering rate in LSCO. JOEL MESOT, ETH Zurich and PSI — An angle-resolved photoemission study of the scattering rate in the normal and superconducting states of the high-temperature superconductor La(2-x)Sr(x)CuO(4) as a function of binding energy and momentum will be presented. We report that, close to optimal doping, the scattering rate scales linearly with binding energy up to a high-energy scale E1. The scattering rate is found to be strongly anisotropic, with a minimum along the nodal direction of the superconducting gap. Since both the degree of anisotropy and the energy dependence of the scattering rate appear to be strongly doping dependent, possible connections to a quantum-critical point will be discussed.

3:42PM D2.00003 Fermi surface of underdoped cuprate revealed by quantum oscillations and Hall effect. CYRIL PROUST, Laboratoire National des Champs Magnétiques Pulses (CNRS) — Despite twenty years of research, the phase diagram of high temperature superconductors remains enigmatic. A central issue is the origin of the differences in the physical properties of these copper oxides doped to opposite sides of the superconducting region. In the overdoped regime, the material behaves as a reasonably conventional metal, with a large Fermi surface [1]. The underdoped regime, however, is highly anomalous and appears to have no coherent Fermi surface, but only disconnected ‘Fermi arcs’ [2]. We have reported the observation of quantum oscillations in the electrical resistance of the oxygen-ordered cuprates, YBa$_2$Cu$_3$O$_{6.5}$ [3] and YBa$_2$Cu$_3$O$_{6.9}$ [4], establishing the existence of a coherent closed Fermi surface at low temperature in the underdoped side of the phase diagram of cuprates, once superconductivity is suppressed by a large magnetic field. The low oscillation frequency reveals a Fermi surface made of small pockets, in contrast to the large cylinder characteristic of the overdoped regime. Moreover, the negative sign of the Hall effect at low temperature reveals that these pockets are electron-like rather than hole-like. We propose that the Fermi surface of these Y-based cuprates consists of both electron and hole pockets, probably arising from a reconstruction of the FS [5].

Work in collaboration with N Doiron-Leyraud, D. LeBoeuf and L. Taillefer from the University of Sherbrooke, J. Levallois and B. Vignolle from the LNCMP, A. Bangura and N. Hussey from the University of Bristol and R. Liang, D. Bonn, W. Hardy from the University of British Columbia.


4:18PM D2.00004 Fermi orbits versus Fermi arcs. NEIL HARRISON, Los Alamos National Laboratory — We consider the effect of a short antiferromagnetic correlation length $\xi$ on the electronic bandstructure of the underdoped cuprates. Starting with a Fermi-surface topology thought to be consistent with that determined from magnetic-quantum-oscillation experiments, we show that a reduced $\xi$ gives an asymmetric broadening of the quasiparticle dispersion, resulting in simulated ARPES data very similar to those observed in experiment. Predicted features include the presence of 'Fermi arcs' close to $k=(\pi/2, \pi/2)$, where $\alpha$ is the in-plane lattice parameter, without the need to invoke a $\delta$-wave pseudogap order parameter. The statistical variation in the $k$-space areas of the reconstructed Fermi-surface pockets causes the quantum oscillations to be strongly damped, even in very strong magnetic fields, in agreement with experiment. (I would like to extend special thanks to the coauthors John Singleton and Ross McDonald and to E. Yelland and L. Taillefer for useful discussions.)

This work is supported by the DOE project Science in 100 tesla and also by the National Science Foundation.
4:54PM D2.00005 Fermi surface and anisotropic scattering in overdoped cuprates. NIGEL HUSSEY, University of Bristol — In the light of recent results detailing the emergence of small Fermi pockets and anomalous Hall coefficients in overdoped cuprates, we review here our measurements on the Fermiology and low temperature transport of cuprates that reside on the other side of the superconducting dome. Analysis of angle-dependent magnetoresistance and Hall coefficient data in $Tl_2Ba_2CuO_{6+x}$ and $La_{2-x}Sr_xCuO_4$ has uncovered a wealth of structure, not only in the (un-reconstructed) Fermi surface in overdoped cuprates, but also in the basal-plane transport scattering rate, in both the elastic and the inelastic channels. A striking correlation between the superconducting transition temperature and the strength of the anisotropic scattering is also revealed suggesting an intimate link between anisotropic scattering and the pairing mechanism itself. Finally, we discuss possible origins of these various anisotropic terms and how they might impact on our understanding of the evolution of the resistivity and the Hall coefficient across the entire cuprate phase diagram.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D3 DMP: Materials Physics in the Fast Lane Morial Convention Center RO2 - RO3

2:30PM D3.00001 The Art and Materials Physics of the Motorcycle. CHARLES M. FALCO, University of Arizona — In 1871 Louis Perreux installed a compact steam engine in a commercial bicycle, and thus produced the world’s first motorcycle. A steam engine was a logical choice, having steadily developed from the work of Savery and Newcomen in the 17th century to the point where Perreux was able to make one small enough to use for this purpose. Unfortunately, it was a technological dead-end the moment it was created, since nine years earlier Alphonse Beau de Rochas had published the description of his four-cycle internal-combustion process. Significantly, the Michaux-Perreux engine produced 1-2 hp in an overall contraption that weighed 88 kg, whereas modern motorcycles produce 200 times more power while weighing only twice as much. Examples I will show illustrate that developments in materials science over the past century are almost entirely responsible for making this possible. After a period of extraordinarily-rapid technological advance, by 1903 essentially all the components of a modern motorcycle were in place, and changes since then have been largely the result of evolutionary refinement in step with advances in materials science, rather than further revolutionary invention. Also, like many other objects of industrial design, motorcycles have played a variety of roles in society over the 137 years since the Michaux-Perreux. I will discuss the interrelationship of the relevant technological, cultural, and aesthetic factors over the past century that have, amongst other things, resulted in standard production motorcycles incorporating such materials as carbon-fiber composites, maraging steels, and “exotic” alloys of magnesium, titanium and aluminum – that can exceed 190 mph straight from the show room floor. For more information see http://www.optics.arizona.edu/sad/aotm.html. Acknowledgment: I am grateful for the contributions of Ulan Guifoyle to our joint work on the Solomon R. Guggenheim’s “The Art of the Motorcycle.”

3:06PM D3.00002 Materials at 200 mph: Making NASCAR Faster and Safer, DIANDRA LESLIE-Pelecky, University of Nebraska — You cannot win a NASCAR race without understanding science. Materials play important roles in improving performance, as well as ensuring safety. On the performance side, NASCAR limits the materials race car scientists and engineers can use to limit ownership costs. “Exotic metals” are not allowed, so controlling microstructure and nanostructure are important tools. Compacted Graphite Iron, a cast iron in which magnesium additions produce interlocking microscale graphite reinforcements, makes engine blocks stronger and lighter. NASCAR’s new car design employs a composite called Tegris$^{TM}$ that has 70 percent of the strength of carbon fiber composites at about 10 percent of the cost. The most important role of materials in racing is safety. Drivers wear firesuits made of polymers that carbonize (providing thermal protection) and expand (reducing oxygen access) when heated. Catalytic materials originally developed for space-based CO$_2$ lasers filter air for drivers during races. Although materials help cars go fast, they also help cars slow down safely—important because the kinetic energy of a race car going 180 mph is nine times greater than that of a passenger car going 60 mph. Energy-absorbing foams in the cars and on the tracks control energy dissipation during accidents. To say that most NASCAR fans (and there are estimated to be 75 million of them) are passionate about their sport is an understatement. NASCAR fans understand that science and engineering are integral to keeping their drivers safe and helping their teams win. Their passion for racing gives us a great opportunity to share our passion for science with them. NASCAR® is a registered trademark of the National Association for Stock Car Auto Racing, Inc. Tegris$^{TM}$ is a trademark of Milliken & Company.

3:42PM D3.00003 Sox and Drugs: Baseball, Steroids and Physics, ROGER TOBIN, Tufts University — The sports world is in an uproar over performance-enhancing drugs. In the United States steroids in baseball have received the most attention, in part because the purported effects are much more dramatic than in any other sport. From 1995-2003 a few players hit home runs at rates 20-50% higher than the best sluggers of the preceding century. Could steroids really increase home-run performance that much? I will describe a model that combines estimates of the physiological effects of steroids, known baseball physics, and reasonable models of batting effectiveness for highly skilled hitters. A 10% increase in muscle mass, which can reasonably be expected from steroid use, increases the speed of a batted ball by 3%. Because home runs are relatively rare events on the tail of a batter’s range distribution, even this modest change in ball speed can increase the proportion of batted balls that result in home runs by 30 – 70%, enough to account for the record-shattering performances of the recent past. I will also describe some of the attention — both welcome and not — that comes to the unsuspecting physicist who wades into such emotionally troubled waters.

4:18PM D3.00004 Zero CTE Glass in the Hubble Space Telescope, JOHNN WOOD, NASA Goddard Space Flight Center — Orbiting high above the turbulence of the earth’s atmosphere, the Hubble Space Telescope (HST) has provided breathtaking views of astronomical objects never before seen in such detail. The steady diffraction-limited images allow this medium-size telescope to reach faint galaxies fainter than 30th magnitude. Some of these galaxies are seen as early as 2 billion years after the Big Bang in a 13.7 billion year old universe. Up until recently, astronomers assumed that all of the laws of physics and astronomy applied back then as they do today. Now, using the discovery that certain supernovae are “standard candles,” astronomers have found that the universe is expanding faster today than it was back then: the universe is accelerating in its expansion. The Hubble Space Telescope is a two-mirror Ritchey-Chrétien telescope of 2.4m aperture in low earth orbit. The mirrors are made of Ultra Low Expansion (ULE) glass by Corning Glass Works. This material allows rapid figuring and outstanding performance in space astronomy applications. The paper describes how the primary mirror was mis-figured in manufacturing and later corrected in orbit. Outstanding astronomical images taken over the last 17 years show how the application of this new technology has advanced our knowledge of the universe. Not only has the acceleration of the expansion been discovered, the excellent imaging capability of HST has allowed ground-breaking research on cosmology, dark matter and dark energy in distant clusters of galaxies. The HST has touched practically every field of astronomy enabling astronomers to solve many long-standing puzzles. It will be a long time until the end of the universe when the density is near zero and all of the stars have long since evaporated. It is remarkable that humankind has found the technology and developed the ability to interpret the measurements in order to understand this dramatic age we live in.
Coherent tunneling of electron and hole spin between two quantum dots using optical spectroscopy [1,2]. In the case of a hole spin, a very large and resonant enhancement or reduction of g-factor is controlled with an applied electric field [3]. This effect arises because of the corresponding enhancement or suppression of the hole wavefunction in the tunnel barrier for the bonding (symmetric) and anti-bonding (anti-symmetric) states, respectively. This effect was discovered for single holes, but also occurs for two-particle states (two holes or 1 hole and 1 electron). Using this effect to identify the symmetry of the wavefunction, we have now found that the energetic order of the bonding and anti-bonding molecular states goes through a reversal as a function of tunnel barrier thickness. That is, the bonding state is the low energy state for a 2nm barrier thickness (as expected in the simple particle-in-a-box model, or the one-band effective mass theory). But for thicknesses larger than 3nm, a transition occurs such that the anti-bonding state becomes the low energy state. This dramatic and non-intuitive effect arises from the spin-orbit interaction.

Monday, March 10, 2008 2:30PM - 4:54PM –
Session D4 DCMP: Probing Spin and Charge States in Semiconductor Quantum Dots and Molecules  Morial Convention Center 206

2:30PM D4.00001 Spin tunneling in optically excited quantum dot molecules: Controlling g-factors with electric field , MATTHEW DOTY, Materials Science and Engineering, University of Delaware — We have recently demonstrated coherent tunneling of electron and hole spin between two quantum dots using optical spectroscopy [1,2]. In the case of a hole spin, a very large and resonant enhancement or reduction of g-factor is controlled with an applied electric field [3]. This effect arises because of the corresponding enhancement or suppression of the hole wavefunction in the tunnel barrier for the bonding (symmetric) and anti-bonding (anti-symmetric) states, respectively. This effect was discovered for single holes, but also occurs for two-particle states (two holes or 1 hole and 1 electron). Using this effect to identify the symmetry of the wavefunction, we have now found that the energetic order of the bonding and anti-bonding molecular states goes through a reversal as a function of tunnel barrier thickness. That is, the bonding state is the low energy state for a 2nm barrier thickness (as expected in the simple particle-in-a-box model, or the one-band effective mass theory). But for thicknesses larger than 3nm, a transition occurs such that the anti-bonding state becomes the low energy state. This dramatic and non-intuitive effect arises from the spin-orbit interaction.

3:06PM D4.00002 Universal Quantum Gates for Two- and Three-Spin Qubits in Coupled Quantum Dots , GUIDO BURKARD, RWTH Aachen University, Germany — The ability to control the exchange coupling between coupled quantum dots allows for quantum gate operations on quantum dot spin qubits. Supplemented with single-spin rotations, the exchange coupling is universal for quantum computation on qubits that are formed by the spin 1/2 of single electrons. If qubits are formed by two spins, the requirement for single-spin rotations is reduced to the presence of a fixed inhomogeneous magnetic field, while for three spins, the exchange coupling is universal on its own. In this talk, we discuss the implementation of universal gate operations for two- and three-spin qubits in coupled quantum dots. In the case of the two-spin singlet-triplet qubit on a double quantum dot, we propose a set of universal gates that can be generated by controlling the electrostatic potential between the two dots without time-dependent control of the tunnel coupling between the dots [1]. This simplification should facilitate the implementation of quantum gates in the systems that are presently studied experimentally. We present explicit gate sequences for single-qubit rotations about two orthogonal axes, and a CNOT gate sequence, completing the universal gate set. Finally, the trade-off between leakage errors and simple operations will be briefly discussed.

3:42PM D4.00003 Nondestructive optical probe of coherent single spin dynamics in a quantum dot , JESSE BEREZOVSKY, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Understanding the coherent dynamics of a single electron spin in a quantum dot (QD) is important for potential applications in solid-state, spin-based quantum information processing. Here, results will be presented focusing on optical detection of a single spin and observation of the temporal evolution of the spin state. First, we demonstrate the detection of a single electron spin in a QD using a continuously averaged magneto-optical Kerr rotation (KR) measurement [2]. In contrast to many other single spin detection schemes, the KR measurement minimally disturbs the system, making it potentially useful for exploring quantum measurement phenomena or spin-photon entanglement. This continuous single QD KR technique is then extended into the time domain using pulsed pump and probe lasers, allowing the observation of the coherent evolution of an electron spin state with nanosecond temporal resolution [3]. This provides a direct measurement of the electron g-factor and spin lifetime, and additionally serves as a sensitive probe of the local nuclear spin environment. Finally, we perform ultrafast coherent optical manipulation of the electron spin state in the QD using the optical Stark effect [4] where an off-resonant optical pulse induces rotations of the spin state through angles up to $\pi$ radians on picosecond timescales.

Yamamoto, Yu. A. Pashkin, and J.S. Tsai. This work has been supported by RIKEN Frontier Research System and CREST-JST.

is pumped incoherently to the upper state and emits photon into the cavity. This work is in collaboration with O. Astafiev, K. Inomata, A.O. Niskanen, T. J. M. Gambetta, Jens Koch, B. R. Johnson, J. A. Schreier, L. Frunzio, D. I. Schuster, A. A. Houck, A. Wallraff, A. Blais, M. H. Devoret, S. M. Girvin and R. J. Schoelkopf, ALEXANDRE BLAIS, Universite de Sherbrooke — Coupling of superconducting qubits to resonant cavities and mechanical oscillators has opened new possibilities for quantum information processing and for the realization of quantum optics in solid-state devices. Together with steady improvements in superconducting qubits [1], this is due to the qubit-resonator coupling which can readily be made very large with respect to all dissipation rates. As a result, these solid-state systems can reach new parameter regimes currently unexplored in atomic based quantum optics [2]. A resonant cavity can also be used as quantum bus allowing entanglement to be generated controllably between qubits coupled to the same cavity, and regardless of the distance separating the qubits [3]. Because of the relatively large size of these cavities, this allows to couple and entangle multiple qubits, opening new avenues for scalable solid-state quantum computation. In this talk, I will review some of the key properties of superconducting qubits and how they can be strongly coupled to various types of resonant cavities. Focusing on superconducting charge qubits coupled to transmission line resonators, I will explain how the quantum state of the qubits can be coherently manipulated and probed by microwave irradiation of the resonator [4]. I will also present some of the recent theoretical proposals for the generation of entanglement in this system [5].

References:

Work done in collaboration with A. Wallraff, M. Devoret, S.M. Girvin, R.J. Schoelkopf and the Yale circuit QED team.

3:06PM D5.00002 Coherent manipulation of quantum information using two Josephson phase qubits coupled to a resonant cavity, MIKA SILLANPAA, National Institute of Standards and Technology — We have taken the first step towards the implementation of circuit quantum-electro dynamics (QED) quantum information processing with Josephson phase qubits. We have observed for the first time a coherent interaction between two phase qubits and an LC cavity formed by a 7 mm long coplanar waveguide resonator at 9 GHz. When either qubit is resonant with the cavity, we observe the vacuum Rabi splitting of the qubit’s spectral line. In a time-domain measurement, we observe coherent vacuum Rabi oscillations between either qubit and the oscillator. Using controllable shift pulses, we have shown coherent transfer of a arbitrary quantum state. We first prepare the first qubit in a superposition state, then this state is transferred to the resonant cavity and then after a short time, we transfer this state into the final qubit. These experiments show that quantum information can be coherently stored and transferred between superconducting quantum bits using a resonant cavity. This opens up new possibilities for performing circuit QED and studying quantum information science.

3:42PM D5.00003 Circuit QED: Coupling Superconducting Qubits via a Cavity Bus on a Chip, JOHANNES MAJER, Yale University, Applied Physics — Circuit quantum electrodynamics is a system, which allows us to do new experiments in quantum optics with a superconducting integrated circuit on a chip. In circuit QED, microwave photons are guided and confined by superconducting transmission lines and cavities, and can then be coherently coupled to a transmon qubit. This system leads to much stronger coupling of the “light” and “matter” than is possible with traditional atomic systems. Making use of that strong coupling it is possible to couple two qubits via the cavity[1]. I will show how one can use the cavity as a coupling bus which provides non-local and non-nearest neighbor coupling. The interaction is mediated by the exchange of virtual rather than real photons, avoiding cavity-induced loss. The same cavity is also used to perform multiplexed control and read-out of the two qubits. The coupling is effectively switchable which allows for time domain transfer of the quantum states between the qubits. [4] Coupling superconducting qubits via a cavity bus, J. Majer, J. M. Chow, J. M. Gambetta, Jens Koch, B. R. Johnson, J. A. Schreier, L. Frunzio, D. I. Schuster, A. A. Houck, A. Wallraff, A. Blais, M. H. Devoret, S. M. Girvin and R. J. Schoelkopf. Nature 449 443 (2007)

4:18PM D5.00004 Single artificial-atom maser, YASUNOBU NAKAMURA, NEC Nano Electronics Research Laboratories — MASERS and lasers usually involve ensemble of atoms to be excited and stimulated for emission. As those atoms are only weakly coupled to the cavity mode, a large number of atoms and strong pumping are needed for lasing in order to overcome the cavity loss and the relaxation of atoms due to spontaneous emission into other modes. However, when the coupling becomes strong even a single atom is enough for lasing, as have been demonstrated with atoms in microwave/optical cavities. We have realized an analogous single artificial-atom maser in a superconducting circuit [1]. Josephson-junction charge qubit is used as an artificial atom with a large dipole. The qubit is coupled to a superconducting Nb coplanar-waveguide resonator at around 10 GHz and with a quality factor of 7600. The coupling strength between the qubit and the resonator is 80 MHz. Population inversion is generated by current injection: A current is injected through a voltage-biased electrode attached to the charge qubit via a highly resistive tunnel junction. In the so-called Josephson-quasiparticle process, the qubit is pumped incoherently to the upper state and emits photon into the cavity. This work is in collaboration with O. Astafiev, K. Inomata, A.O. Niskanen, T. Yamamoto, Yu. A. Pashkin, and J.S. Tsai. This work has been supported by RIKEN Frontier Research System and CREST-JST.

4:54PM D5.00005 Process Tomography of Quantum Memory in a Josephson Phase Qubit. MATTHEW NEELEY, University of California, Santa Barbara — Quantum memory that can protect qubit states against decoherence is an important piece of a scalable quantum computing architecture. Coupling a qubit to a high-Q harmonic oscillator memory element is one example, but many other quantum systems could serve this role. We have used an atomic two-level state (TLS) in the amorphous AlOx tunnel barrier of a Josephson phase qubit as a prototype quantum memory element. The frequency-tunability of the phase qubit allows us to switch on and off the qubit-TLS coupling and thereby transfer arbitrary qubit states into the TLS, store them for some time and recall them later. We performed quantum process tomography to completely characterize the memory operation and the errors that occur during the state transfer and recall. The overall process fidelity is 78%. The dominant operator-sum errors are dephasing-like (~12%) and relaxation-like (~9%), consistent with the measured $T_1$ and $T_2$ of the TLS.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D6 FIAP DPOLY: Long-Distance Charge Transfer in Biological Systems Morial Convention Center RO4

2:30PM D6.00001 Theory of Electron Transfer and Transport Pathways in Biomolecules. DAVID BERATAN, Duke University — Electron transfer in proteins and nucleic acids occurs over large distances by a combination of short and long range tunneling mechanisms. Electron tunneling is facilitated by virtual oxidized and reduced states of the bridging macromolecule, and theoretical analysis reveals how a macromolecule’s fold, energetics, and fluctuations influence the electron-transfer kinetics. Recent studies of protein electron transfer indicate when and why electron tunneling kinetics is sensitive to the structure of the protein’s tunneling pathways. Electron transfer across protein-protein interfaces involves thin structured water layers that play a key role in tunneling mediation as well. Tunneling analysis that takes the dynamical fluctuations of the macromolecules into explicit account provides a unified view that links structure and function in protein electron transfer. In the case of DNA electron transport, a critical role is found for structural fluctuations and transport mediated by carrier injection to intervening bases, even at very short distances.

3:06PM D6.00002 Long-Range Electron Transfer through Proteins and Solvents. JAY WINKLER, California Institute of Technology — Reactions in which electrons tunnel long distances from donors (D) to acceptors (A) pervade solid-state physics, chemistry and biology. Theory suggests that the barriers to these tunneling processes depend strikingly on the composition and structure of the intervening medium. Poor coupling across nonbonded interfaces produces a strong bias in favor of covalent and hydrogen-bonded pathways between redox sites in proteins. The coupling disparity between bonded and nonbonded interfaces accounts in large part for the finding that protein electron-transfer rates do not exhibit a uniform dependence on distance, but instead depend critically on the composition of the medium between redox sites. Rates at a single D-A separation can differ by more than one order of magnitude in D-A distances that differ by much as 0.5 nm can produce identical rates. Our investigations of electron tunneling through proteins and solvents are aimed at elucidating the factors that determine long-range D-A couplings.

3:42PM D6.00003 Correlated electron and proton transport in cytochrome c oxidase: Coulomb proton pump with kinetic gating1, ALEXEI STUCHEBRUKHOV, University of California at Davis — I will discuss correlated transport of electrons and protons in cytochrome c oxidase, the terminal enzyme in the respiratory electron transport chain of aerobic organisms. This enzyme catalyzes the reduction of atmospheric oxygen to water in our cells, and utilizes the free energy of oxygen reduction for the creation the proton gradient by pumping protons across the membrane. The proton gradient subsequently drives the synthesis of ATP. The details of the mechanism of this redox-driven proton pump are unknown. Computer simulations and theoretical modeling point to a possible mechanism of this biological molecular machine in which electron transport is coupled to proton translocation.
3:06PM D7.00002 Theory of swimming filaments in viscoelastic media. HENRY FU, Brown University — Microorganisms often encounter and must move through complex media. What aspects of propulsion are altered when swimming in viscoelastic gels and fluids? Motivated by the swimming of sperm through the mucus of the female mammalian reproductive tract, we examine the swimming of filaments in nonlinearly viscoelastic fluids. We obtain the swimming velocity and hydrodynamic force exerted on an infinitely long cylinder with prescribed beating pattern. We apply these results to study the swimming of a simplified sliding-filament model for a sperm flagellum. Viscoelasticity tends to decrease swimming speed. The viscoelastic response of the fluid can change the shapes of beating patterns, and changes in the beating patterns can even lead to reversal of the swimming direction.

3:42PM D7.00003 Undulatory swimming in a viscoelastic fluid. LISA FAUCI, Tulane University — Mammalian spermatozoa encounter complex, non-Newtonian fluid environments as they make their way through the female reproductive tract. The beat form realized by the flagellum varies tremendously along this journey. We will present recent progress on the development of computational models that couple the internal force generation of undulating flagella with the external dynamics of a complex fluid. An immersed boundary framework is used, with the complex fluid represented either by a continuum Oldroyd-B model, or a Newtonian fluid overlaid with discrete viscoelastic elements.

4:18PM D7.00004 Large and limbless: the locomotion of snakes. DAVID HU, Courant Institute — In efforts to understand snake locomotion, we consider one of their various gaits. By contracting and extending their bodies unidirectionally like a slinky, large snakes propel themselves in a straight line. In a combined experimental and theoretical investigation, we here report on the dynamics of a boa constrictor alongside the analysis of an n-linked extensible crawler model. Constraints on their locomotion are quantified and discussed, such as the elasticity, frictional anisotropy and abrasive wear of their skin. Also presented are certain snake behaviors that culminate in their tying themselves into knots.

4:54PM D7.00005 Biological and robotic movement through granular media. DANIEL GOLDMAN, Georgia Institute of Technology — We discuss laboratory experiments and numerical simulations of locomotion of biological organisms and robots on and within a granular medium. Terrestrial locomotion on granular media (like desert and beach sand) is unlike locomotion on rigid ground because during a step the material begins as a solid, becomes a fluid and then re-solidifies. Subsurface locomotion within granular media is unlike swimming in water for similar reasons. The fluidization and solidification depend on the packing properties of the material and can affect limb penetration depth and propulsive force. Unlike aerial and aquatic locomotion in which the Navier-Stokes equations can be used to model environment interaction, models for limb interaction with granular media do not yet exist. To study how the fluidizing properties affect speed in rapidly running and swimming lizards and crabs, we use a trackway composed of a fluidized bed of of 250 μm glass spheres. Pulses of air to the bed set the solid volume fraction 0.50 < φ < 0.63; a constant flow rate Q below the onset of fluidization (at Q = Qf) linearly reduces the material strength (resistance force per depth) at fixed φ for increasing Q. Systematic studies of four species of lizard and a species of crab (masses ≈ 20 grams) reveal that as Q increases, the average running speed of an animal decreases proportionally to √(M/A - const*(1 - Q/Qf)) where M is the mass of the animal and A is a characteristic foot area. While the crabs decrease speed by nearly 75% as the material weakens to a fluid, the zebra tailed lizard uses long toes and a plantigrade foot posture at foot impact to maintain high speed (≈ 1.5 m/sec). We compare our biological results to systematic studies of a physical model of an organism, a 2 kg hexapedal robot SandBot. We find that the robot speed sensitively depends on φ and the details of the limb trajectory. We simulate the robot locomotion by computing ground reaction forces on a numerical model of the robot using a soft-sphere Molecular Dynamics code.

3Work supported by a Burroughs Wellcome Fund CASI award

Monday, March 10, 2008 2:30PM - 5:30PM — Session D8 DFD GSNP: Focus Session: Granular Flows: Vibrated Morial Convention Center RO6

2:30PM D8.00001 Particle kinematics in a 3-dimensional vibration-fluidized granular medium. HONG-QIANG WANG, NARAYANAN MENON, University of Massachusetts Amherst — We report a study by high speed video imaging of particle motions in the bulk of a three dimensional granular gas. We fluidise with intense vertical vibration, delrin spheres of diameter, d=1.6 mm confined in a 3-dimensional volume (32d)3. We isolate particles moving in a thin slice of this volume by illuminating with a laser sheet. We have developed a new algorithm to track with sub-pixel precision particles that are only partially illuminated or eclipsed by other particles. We will present data in the low-volume fraction regime for spatial profiles of the the kinetic temperature and number density, as well as for the velocity distribution. These results will be compared to predictions from hydrodynamic models.

3This work was supported through NASA NNC05AA35A and NSF DMR 0606216.

2:42PM D8.00002 Heating mechanism affects equipartition in a binary granular system. NARAYANAN MENON, HONGQIANG WANG, Dept of Physics, U. of Massachusetts — Two species of particles in a binary granular system typically do not have the same mean kinetic energy, in contrast to the equipartition of energy required in equilibrium. We investigate the role of the heating mechanism in determining the extent of this non-equipartition of kinetic energy. In most experiments, different species of particle are unequally heated at the boundaries. We show by event-driven simulations that this differential heating at the boundary influences the level of non-equipartition even in the bulk of the system. This conclusion is fortified by studying a numerical model and a solvable stochastic model without spatial degrees of freedom. In both cases, even in the limit where heating events are rare compared to collisions, the effect of the heating mechanism persists.

2We gratefully acknowledge support from NASA NNC05AA35A and NSF DMR 0606216

2:54PM D8.00003 Energy fluctuation, diffusivity and mobility in a 2D vibrated granular packing. ERIC CLEMENT, RIM HARICH, ESPCI -Université Paris 6, NICOLAS VANDEWALLE, GEOFFROY LUMAY, GRASP-Université Li`ege — We present an experimental realization of a 2D vibrated granular packing. The new agitation method allows a spatially non synchronized influx of energy and the study of the vibrated packing at steady state. By image analysis of fast-camera movies, we obtain the velocity fluctuation spectra at different vertical levels and then, we separate the agitation velocities from the velocity fluctuations corresponding to the “thermalized” degrees of freedom. By measuring the corresponding particle diffusivities, we show that, in spite a large heterogeneity and anisotropy of the vibration, a relation between diffusivity and “thermalized” kinetic energy can be identified. We relate this type of fluctuation-dissipation relation to the mobility of macroscopic intruders of different sizes and weight moving in the vibrated granular packing.

1PMMH-ESPCI is the UMR 7636 of the CNRS.
steady rotation, the critical angle of the first failure decreases slightly from the steady-state value due to the lack of an established steady-state force network.

external vibrations on this "unjamming" transition. While larger vibrations destabilize the pile and decrease the maximum angle of repose, small vibrations lead 

Madison University — We present work on a 2D free surface granular flow experiment under vertical vibration. The experiment consists of photoelastic grains in 

is evidenced at low vibration energy, both for glass beads and natural sand. Conversely, shear thinning is observed at high agitation.

coefficients between the base and the granular layer under sustained and controlled vibrations. A shear thickening regime characteristic of dense granular flows 

an exponentially nonlinear diffusion equation is derived theoretically that describes the evolution of the deposit shape. A self-similar parabolic shape (the "granular droplet") and 

Paris, France, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, ARGONNE, IL60439, USA — The influence of controlled vibrations 

MSC, UMR 7057 (CNRS), Univ. Paris 7, JOSE LANUZA, BRUNO ANDREOTTI, PMMH, UMR7636 (CNRS), ESPCI Univ. P6-P7, 10 Rue Vauquelin, 75005 

Research Supported by Army Research Office

4:06PM D8.00007 Numerical Study of Particle Damping Mechanism in Piston Vibration System via Particle Dynamics Simulation, XIAN-MING BAI, BINYO SHAH, LEON KEER, JANE WANG, RANDALL SNURR, Northwestern University — Mechanical damping systems with granular particles as the damping media have promising applications in extreme temperature conditions. In particle-based damping systems, the mechanical energy is dissipated through the inelastic collision and friction of particles. In the past, many experiments have been performed to investigate the particle damping problems. However, the detailed energy dissipation mechanism is still unclear due to the complex collision and flow behavior of dense particles. In this work, we use 3-D particle dynamics simulation to investigate the damping mechanism of an oscillating cylinder piston immersed in millimeter-size steel particles. The time evolution of the energy dissipation through the friction and inelastic collision is accurately monitored during the damping process. The contribution from the particle-particle interaction and particle-wall interaction is also separated for investigation. The effects of moisture, surface roughness, and density of particles are carefully investigated in the simulation. The comparison between the numerical simulation and experiment is also performed. The simulation results can help us understand the particle damping mechanism and design the new generation of particle damping devices.

4:18PM D8.00008 Breaking of granular jams with mechanical shocks, KE CHEN, ANDREW HARRIS, JOHN DRASKOVIC, PETER SCHIFFER, Department of Physics, Penn State University — We studied the brief granular flows initiated by breaking the jamming in a hopper using mechanical shocks. Jamming near the orifice of a hopper prevents granular materials from flowing spontaneously under gravity. Controlled mechanical shocks were applied from the bottom of the hopper to break the jamming and to initiate brief flows. The magnitude and the duration of the flows were measured. Preliminary results show that the probability of initiating a flow increases with the intensity of the shock, and reaches almost 100% at the highest shock intensities. We also investigated the flow probability as a function of the ratio between the diameters of the orifice and the bead. Statistical characteristics of the flow magnitude and duration evolve with shock intensity as well as the ratio between the diameters of the orifice and the bead. This research was supported by the NASA through grant NAG3-2384 and the NSF REU program through grant DMR 0305238.

4:30PM D8.00009 Spreading of a granular droplet, ERIC CLEMENT, PMMH, UMR7636 (CNRS), ESPCI Univ. P6-P7, 10 Rue Vauquelin, 75005 Paris, France, IVAN SANCHEZ, Centro de Fisica, IUC, Apartado Postal 21827, Caracas 1020-A, Venezuela, FRANCK RAYNAUD, MSc, UMR 7057 (CNRS), Univ. Paris 7, JOSE LANUZA, BRUNO ANDREOTTI, PMMH, UMR7636 (CNRS), ESPCI Univ. P6-P7, 10 Rue Vauquelin, 75005 Paris, France, IGOR ARANSON, Materials Science Division, Argonne National Laboratory, Argonne, IL60439, USA — The influence of controlled vibrations on the granular rheology is investigated in a specifically designed experiment in which a granular film spreads under the action of horizontal vibrations. A nonlinear diffusion equation is derived theoretically that describes the evolution of the deposit shape. A self-similar parabolic shape (the "granular droplet") and a spreading dynamics are predicted that both agree quantitatively with the experimental results. The theoretical analysis is used to extract effective friction coefficients between the base and the granular layer under sustained and controlled vibrations. A shear thickening regime characteristic of dense granular flows is evidenced at low vibration energy, both for glass beads and natural sand. Conversely, shear thinning is observed at high agitation.

4:42PM D8.00010 2D granular avalanches with imposed vibrations, BRIAN UTTER, DAN AMON, James Madison University — We present work on a 2D free surface granular flow experiment under vertical vibration. The experiment consists of photoelastic grains in a 2D circular drum which is rotated at a constant rate (f < 1 mHz). We measure time series of the slope, particle trajectories, and image the bulk force network. Avalanche and build-up distributions exhibit a power-law dependence as previously observed. We then vibrate the drum vertically to determine the effect of external vibrations on this "unjamming" transition. While larger vibrations destabilize the pile and decrease the maximum angle of repose, small vibrations lead to a strengthening of the pile and tend to increase the critical angle of failure. In the absence of vibration, when the drum is rotated opposite the direction of steady rotation, the critical angle of the first failure decreases slightly from the steady-state value due to the lack of an established steady-state force network.
4:54PM D8.00011 Bouncing trimer¹. STEPHANE DORBOLO, FNRS, NICOLAS VANDEWALLE, University of Liege, GRASP TEAM — Trimers are composed of three stainless steel beads (1 cm of diameter) forming a solid equilateral triangle (2.5 cm of side). They are placed on a plate of an electromagnetic shaker. The system is shaken vertically. According to the acceleration, the trimer may spin, jump once every two periods or even every three periods. Between these stable regimes, the system is chaotic. By measuring the time delay between two successive shocks (beam-plate), a mapping of the different regimes has been constructed. The spinning, 2-period and 3-period orbits occurs for the same acceleration whatever the frequency. However, the spin speed has been measured with respect of the frequency.

1SD thanks FNRS for financial support

5:06PM D8.00012 Dynamics of a single particle on a 2D driven granular lattice. JEFFREY OLAFSEN, KRISTIN COMBS, Department of Physics, Baylor University, G. WILLIAM BAXTER, Physics Department, Penn State Erie, The Behrend College — Previous measurements have demonstrated interesting behavior in a novel bi-layer granular gas experiment of mechanically shaken particles. The results are of importance because the two layers are in “thermal contact” and yet have very different dynamical behaviors. The lower layer of particles demonstrates velocity statistics that are strongly correlated and non-Gaussian, while the upper layer of particles concurrently demonstrates a lack of correlations and Gaussian velocity statistics. Details of the collisions within each layer (intralayer) and between the layers (interlayer) are clearly of interest to understand the simultaneous behavior. Measurements are made for a single particle in the upper layer to examine the effects of interlayer collisions. In addition, velocity statistics in both layers are analyzed to determine effects of the sideways.

5:18PM D8.00013 Structure and dynamics of a vibrated granular bead-chain. KEVIN SAFFORD, ARSHAD KUDROLLI, Clark Univ. Physics Dept., YACOV KANTOR, Tel Aviv Univ. Physics Dept., MEHRAN KARDAR, MIT Physics Dept. — We investigate the dynamics of a vibrated granular bead-chain with experiments and numerical simulations of random-walk models of polymers. Experiments are conducted with a chain composed of hollow 3 mm steel beads connected by flexible links confined to move on a 300 mm diameter rough circular bed. Observations made with digital imaging. We analyze the radius of gyration $R_g$, the structure factor of the chain configurations, and the diffusion of the center of mass. We find that $R_g$ and the structure factor scale with the exponent $\nu \sim 3/4$, consistent with the two dimensional self-avoiding random-walk model. Further, we observe confinement effects in the scaling of $R_g$ as the chain length increases relative to the size of the container. We perform simulations of non-self-avoiding walks confined to the same sized domain and find good agreement with experiment. The simulations show confinement effects dominate over self-avoided crossings in the experiments even when the length of chain is smaller than system size. We then experimentally examine the chain dynamics and find that the center of mass diffusion scales inversely as the length of the chain, consistent with the Rouse model of polymers. We observe an exponential decay in the dynamical structure factor and compare this exponent with the measurement of the center of mass diffusion.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D9 DFD: Focus Session: Turbulence Morial Convention Center RO7

2:30PM D9.00001 Turbulent Viscosity Coefficient in 3-Dimesional Turbulence. HIROSHI SHIBATA, Sojo University — A new model for the large-eddy simulation (LES) is proposed. The LES has been accepted as the standard formalism for calculating observables concerning turbulence. In the application of the LES, several models are chosen. The purpose of the present paper is for us to propose one of the most physical models. The LES is usually written down as

$$\frac{\partial U_i}{\partial t} + (\vec{U} \cdot \nabla)U_i = - \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu_0 \Delta U_i - \frac{\partial Q_{ij}}{\partial x_j}. \quad (2)$$

The above equation is rewritten as

$$\frac{\partial U_i}{\partial t} + (\vec{U} \cdot \nabla)U_i = - \frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \Delta U_i \quad (3)$$


2:42PM D9.00002 Exploring the dynamics of the velocity gradient tensor. MARCO MARTINS AFONSO, CHARLES MENEVEAU, Dept. of Mech. Engineering - Johns Hopkins University - Baltimore, MD — The dynamics of the velocity gradient tensor is investigated by means of analytical and numerical computations. Our starting point is the Lagrangian evolution equation of this tensor and a model for the pressure Hessian and viscous term proposed in Chevillard and Meneveau (Phys. Rev. Lett. 97, 174501, 2006). The model is based on the Recent Fluid Deformation (RFD) closure, which was introduced in order to overcome the unphysical finite-time blowup of the Restricted Euler model that neglects anisotropic pressure Hessian effects. Using matrix exponentials, the RFD closure takes into account both the geometry and the dynamics of the recent history of the deformation of a fluid particle, and requires the specification of a decorrelation time scale $\tau$. When this time scale is chosen too short (or, equivalently, the Reynolds number is too high), unphysical statistics are observed in the model. In order to understand this model in greater detail, the original, full matrix-exponential-based model is compared with its power- series expansion for small $\tau$. In particular, the time evolution in the so-called $R-Q$ plane is studied for the two approaches, and also, the effects of adding a Gaussian white noise are examined.

2:54PM D9.00003 The Generalized Fractal Dimensions of a 2-D Compressible Turbulence¹. JASON LARKIN, WALTER GOLDBURG, University of Pittsburgh, MAHESH BANDI, Los Alamos National Laboratory — Steady-state turbulence is generated in a tank of water 1m x 1 m x 0.3 m and the trajectories of particles floating on the surface are tracked in time. Initially the floaters are uniformly distributed. As time goes on they coagulate and form a fractal structure. The surface pattern reaches a steady state in approximately $t^* = 1$ s. In the time interval $0 \leq t < 2t^*$, measurements are made of the generalized fractal dimensions $D_q(t)$ of the floating particles starting with the uniform distribution $D_0(0) = 2$. In the steady state, the pattern formed by the floaters continues to fluctuate at a time scale dictated by the underlying turbulent flow. This time scale is also of the order of 1 s. To understand the origin of the coagulation phenomenon, one must remember that the floaters form a compressible system, unlike the water molecules that drive them. The time evolution of the $D_q(t)$ are measured for a range of $q$ less than 10. The coagulated particles form into string-like structures having values of $D_q$ ranging down to approximately 1.5.

¹Funding from the National Science Foundation
3:06PM D9.00004 Particle Dynamics in Turbulence. HAITAO XU, Max Planck Institute for Dynamics and Self-Organization — The interaction between particles and turbulence features in many environmental and engineering problems, e.g., the formation of rain, the dispersion of particulate pollutants, and sedimentation in rivers and oceans. In addition, tracer particles are routinely used in scientific research to study the flow itself. Understanding the behavior of particles in turbulent flows is not only an important practical problem, but also an intriguing scientific challenge. Our group has developed a three-dimensional Lagrangian Particle Tracking (LPT) system. Using high speed CMOS cameras, the system is capable of following simultaneously hundreds of particles in a turbulent flow with Taylor microscale Reynolds numbers \( R_\lambda \) up to \( 10^5 \). The LPT measurements provide both single- and multi-particle statistics following Lagrangian trajectories, at temporal resolutions better than the Kolmogorov time scales of the turbulence. Due to its ability to follow individual particles, the LPT system is an ideal tool to study the behavior of non-tracer particles in turbulence. The inertial particles have density different from the fluid, but size smaller than the Kolmogorov length scale of turbulence. On the other hand, neutrally buoyant particles with size larger than the Kolmogorov scale behave very differently from inertial particles. We will present results from both cases.

3:42PM D9.00005 Craig’s XY-distribution and the statistics of Lagrangian power in two-dimensional turbulence.1. COLM CONNAUGHTON, University of Warwick, MAHESH BANDI, Los Alamos National Laboratory — We study the probability distribution function (PDF) of injected power in numerical simulations of stationary 2D turbulence in the Lagrangian frame. The simulation mimics an electromagnetically driven fluid layer, a well-documented system for generating 2D turbulence in the laboratory. The forcing and velocity fields in the numerics are close to Gaussian, but the injected power PDF is sharply peaked at zero (suggesting a singularity) with asymmetric exponential tails. Large positive fluctuations are more probable than large negative ones leading to a net positive mean energy input. The main features of the power distribution are well described by Craig’s XY distribution for the PDF of the product of two correlated normal variables. We show that the power distribution should exhibit a logarithmic singularity at zero and decay exponentially for large absolute values of the power. We calculate the asymptotic behaviour and express the asymmetry of the tails in terms of the correlation coefficient of the force and velocity and compare the measured PDFs with theoretical calculations.

3:54PM D9.00006 Multiscale Sample Entropy of 2D Decaying Turbulence. ILDOO KIM, University of Pittsburgh, MATTHEW SHTRAHMAN, Western Pennsylvania Hospital, XIAO-LUN WU, University of Pittsburgh — Kolmogorov-Sinai entropy has been used to quantify degrees of complexity of spatiotemporally chaotic systems. However, it is not always convenient to implement in real experiments. Recently a Multiscale Sample Entropy (MSE) measure has been proposed, which allows easier analyses of time series. In this study, we have generated decaying turbulence in a two-dimensional soap film and have measured velocity fluctuations as functions of time and downstream distance using a laser Doppler velocimeter. We performed MSE analysis and found there is a time scale \( \tau_0 \) at which the MSE is maximized. The value of \( \tau_0 \), which correlates well with the large-eddy turn-over time, gets larger as turbulence decays. Other aspects of 2D turbulence are also analyzed using the velocity time series.

4:06PM D9.00007 Conformal invariance in two-dimensional turbulence. GUIDO BOFFETTA, University of Torino, Italy, DENIS BERNARD, Ecole Normale Superieure, Paris, ANTONIO CELANI, Institut Pasteur, Paris, GREGORY FALKOVICH, Weizmann Institute, Israel — We show that some features of two-dimensional turbulence display conformal invariance. In particular, the statistics of vorticity clusters in the inverse cascade is equivalent to that of critical percolation, one of the simplest universality classes of critical phenomena. Vorticity isolines are therefore described by Stochastic Loewner Equation curves SLE\(_c\). This result is generalized to a class of 2d turbulent systems, including Surface Quasi-Geostrophic turbulence (which corresponds to SLE\(_c\)) and Charney-Hasegawa-Mima turbulence. The picture emerging from our results is that conformal invariance may be expected for inverse cascades in two-dimensions therefore opening new perspectives in our understanding of 2d turbulent flows. References: D. Bernard, G. Boffetta, A. Celani, and G. Falkovich, Nature Physics 2 124 (2006) D. Bernard, G. Boffetta, A. Celani, and G. Falkovich, Phys. Rev. Lett. 98 024501 (2007)

4:18PM D9.00008 Mixing and entrainment of oceanic overflows: Implications for global climate evolution. ROBERT ECKE, JUN CHEN, PHILIPPE ODIER1, MICHAEL RIVERA, Los Alamos National Laboratory — Oceanic overflows are important elements of the Earth’s global thermohaline circulation but the mixing and entrainment that occur for such overflows is poorly understood. In particular, as overflow water moves down an inclined slope its stability is governed by the competition between stratification, which stabilizes the flow, and vertical shear, which tends to destabilize the flow. The properties of our laboratory experiment are designed to mimic oceanic overflows to the extent achievable on laboratory-accessible length scales. The flow exits a nozzle and flows along an inclined plane such that there is gravitational forcing of the flowing gravity current. Velocity and density fields are measured simultaneously using particle image velocimetry and planar laser induced fluorescence. The flow structure and dynamics of mixing at different downstream locations are investigated for a different levels of stratification and shear. The role of turbulence is examined by comparing cases of turbulent and laminar gravity currents. The implication of these results for ocean simulations and for understanding global climate are discussed.

1permanent address: ENS Lyon, France

4:30PM D9.00009 Experimental Investigation of Homogeneity, Isotropy, and Circulation of the Velocity Field in Buoyancy-Driven Turbulence. QUAN ZHOU, Department of Physics, the Chinese University of Hong Kong, CHAO SUN, Department of Applied Physics, University of Twente, KEQING XIA, Department of Physics, the Chinese University of Hong Kong — We present a direct multipoint velocity measurements of the 2D velocity field in the central region of turbulent Rayleigh-Bénard convection. The local homogeneity and isotropy of the velocity field are tested using a number of criteria and are found to hold to an excellent degree. The distribution of \( \Gamma_r \) is found to depend on the scale \( r \), reflecting strong intermittency. Besides, the slight asymmetry of the distribution tails reflects the fact that the velocity circulation structure functions (CSFs) are able to capture anisotropic coherent structures, such as thermal plumes, more effectively than longitudinal structure functions (LSFs) and transversal structure functions (TSFs). It is further found that velocity circulation has the same anomalous scaling exponents as LSFs and TSFs for low-order moments \( \langle p \rangle < 5 \). Whereas, for high-order moments \( \langle p \rangle > 5 \), the anomalous scaling exponents for circulation are found to be systematically smaller than those of LSFs and TSFs.

1This work was supported by the Hong Kong RGC (Grant Nos. CUHK 403705 and 403806).
4:42PM D9.00010 Flow mode transitions in turbulent thermal convection¹, HENG-DONG XI, KE-QING XIA, The Chinese University of Hong Kong — We report an experimental study of structures and dynamics of the large-scale mean flow in Rayleigh-Bénard convection cells with aspect ratio (Γ) 1, 1/2 and 1/3. It is found that both a single circulating roll flow structure and two vertically stacked counter-rotating rolls exist in the three aspect ratio cells. The average percentage of time that the large-scale mean flow spends in the single-roll mode (SRM) and the double-roll mode (DRM) are 87.1% and 0.8% for Γ = 1; 69.5% and 7.9% for Γ = 1/2; and 26.7% and 34.1% for Γ = 1/3. Several routes of transitions among the different flow modes are identified. In addition, fluctuations in the flow structures are found and their relative weights are determined. We also show direct evidence that the SRM is more efficient for heat transfer than the DRM. Although the difference is very small, it shows how changes in internal flow state can manifest in the global transport properties of the system. It is also found that the time interval between successive flow mode transitions has an exponential distribution, suggesting a Poisson process for the underlying dynamics. The duration of the flow mode transition is found to be log-normally distributed.

¹This work was supported by the Research Grants Council of Hong Kong under Grant No. CUHK403705 and CUHK403806.

4:54PM D9.00011 The properties of elastic turbulence in semi-dilute polymer solutions, YONGGUN JUN, Physics of Complex Systems, Weizmann Institute of Science, VICTOR STEINBERG — We studied elastic turbulence in Karman swirling flow of semi-dilute polymer solution. The concentrations of polymer solution used in the experiment were 100, 300, 500, 700, and 900 ppm, and the velocity fields to calculate the rms of the gradients of the tangential velocity, \( \omega_{rms} \), were obtained using PIV. First we checked the saturation of \( \omega_{rms} \) in the bulk, which represents the saturation of elastic stress. We found that \( \Omega_{bulk} = \omega_{rms} \tau \) saturates and approaches to unitary value as the polymer concentration increases. Here \( \tau \) is the longest polymer relaxation time. Also we studied existence of the velocity boundary layer which is related to boundary layer of elastic stresses of elastic turbulence. The thickness of the boundary layer is the decreasing function of polymer concentration near the rotating upper plate but independent of concentrations near the wall.

5:06PM D9.00012 Geometry of plane Couette flow transitional turbulence, PREDRAG CVITANOVIC, JOHN GIBSON, JONATHAN HALCROW, Georgia Tech — We propose to use a hierarchy of exact unstable invariant solutions of the Navier-Stokes equations — corresponding to the recurrent coherent structures observed in experiments — to construct a description of the spatio-temporally chaotic dynamics of turbulent fluid flows as a walk through the space of such structures. This description should allow us to obtain quantitative predictions of transport properties of fluid flows such as bulk flow rate and mean wall drag.

5:18PM D9.00013 The heat transfer of water-based Al₂O₃ nanofluid in turbulent Rayleigh-Bénard convection¹, SHENG-QI ZHOU, RUI NI, KE-QING XIA, Dept. of Physics, The Chinese University of Hong Kong, Hong Kong — We report experimental measurements of the convective heat transfer in water-based Al₂O₃ nanofluid in a cylindrical convection cell, which has 19 cm in both height and diameter. The nanofluid has been supplied by Nanophase Technologies Inc. with an initial volume fraction (φ) 22%. It has been diluted into deionized water to obtain nanofluid of low volume fraction. The nominal diameter of Al₂O₃ particle is 45 nm. At the fixed heating power, \( Q = 500W \), it has been found that the convective heat transfer coefficient (h = Q/\( \Delta T \)) decreases to 2% when φ varies from 0.03% to 1.1%. At φ = 1.1%, we have measured the Nusselt number (Nu) as a function of Rayleigh number (Ra). It has been found that Nu of nanofluid collapses on the Nu ∼ Ra scaling curve of pure water at higher Ra (4 × 10⁹ to 1 × 10¹⁰). While the deterioration of convective heat transfer has been observed at lower Ra (8 × 10⁸ to 4 × 10⁹), and the deterioration becomes more pronounced with decreasing Ra. Additional measurement on the thermal and flow structures is in progress to understand the convective heat transfer in nanofluid.

¹Work supported by the CUHK direct grant 2060309 and United College grant CA11096.

Monday, March 10, 2008 2:30PM - 5:06PM — Session D10 DMP: Focus Session: Hybrid Magnetic-Superconducting Systems I Morial Convention Center R08

2:30PM D10.00001 Odd-frequency pairing state in superconducting junctions, YUKIO TANAKA, Nagoya University — We have theoretically studied the induced odd-frequency pairing states in ballistic normal metal/superconductor (N/S) junctions where a superconductor has even-frequency symmetry in the bulk. We demonstrate that the pair amplitude in the junction has an admixture of an odd-frequency component due to the breakdown of translational invariance near the N/S interface [1]. We have also studied about the proximity effect in junctions between diffusive normal metals (DN) and superconductors. It is revealed for spin-triplet superconductor that the resulting symmetry in DN is always odd-frequency component due to the breakdown of translational invariance near the N/S interface [1]. We have also studied about the proximity effect in junctions between diffusive normal metals (DN) and superconductors. It is revealed for spin-triplet superconductor that the resulting symmetry in DN is always odd-frequency component due to the breakdown of translational invariance near the N/S interface [1]. We have also studied about the proximity effect in junctions between diffusive normal metals (DN) and superconductors. It is revealed for spin-triplet superconductor that the resulting symmetry in DN is always odd-frequency component due to the breakdown of translational invariance near the N/S interface [1]. We have also studied about the proximity effect in junctions between diffusive normal metals (DN) and superconductors. It is revealed for spin-triplet superconductor that the resulting symmetry in DN is always odd-frequency component due to the breakdown of translational invariance near the N/S interface [1].


3:06PM D10.00002 Superfluid density in the ferromagnetic layers of superconductor-ferromagnet hybrid structures, THOMAS LEMBERGER, MICHAEL HINTON, ADAM HAUSER, JULIAN HETEL, FENGYUAN YANG, JULIA MEYER, The Ohio State University — We have measured the areal superfluid density of superconductor-ferromagnet bilayers and trilayers. Samples are made by sputtering Nb and Ni films sequentially in an ultrahigh vacuum chamber with base pressure <10⁻¹⁰ torr. Interfaces are cleaner when Ni is sputtered onto Nb for reasons related to disorder at the initial growth of Nb films. Superfluid density is measured using a low-frequency (50 kHz) two-coil technique with coils on opposite sides of the sample. These measurements provide the true \( T_C \), i.e., the temperature below which superfluid exists. We find a nonmonotonic dependence of \( T_C \) on ferromagnetic layer thickness, in agreement with resistive measurements of \( T_C \). The superfluid density is also nonmonotonic. Even at large ferromagnetic layer thicknesses where \( T_C \) is essentially constant, the areal superfluid density continues to increase, indicating that superfluid extends deeply into the ferromagnet layers. We will discuss these measurements in the context of theory of the superconductor-ferromagnet proximity effect.
3:18PM D10.00003 Study of Inverse Proximity Effect in Ferromagnet/ Superconductor Bilayers Using a Sagnac Interferometer\(^1\), JING XIA, Stanford University, A. PALEVSKI, Tel Aviv University, A. KAPITULNIK, Stanford University — It was recently proposed theoretically that ferromagnetic order can be induced in the superconductor in a ferromagnet/superconductor \((S/F)\) bilayer structure through a so-called inverse proximity effect. The proposal predicts a sizable magnetic moment in the \(S\) layer that couples antiferromagnetically to the moment in the \(F\) layer due to Cooper pairs near the interface formed with one electron in the \(F\) layer and one in the \(S\) layer. The induced magnetic moment is expected to penetrate the superconductor over a size of the Cooper pairs, i.e. \(\xi_s\). In order to directly test this interesting scenario, we fabricated \(Ni/Pb\) and \(Ni/Al\) bilayer samples and probed the possible induced magnetic moments in the \(S\) layer through high resolution Surface Magneto Optical Polar Kerr Effect (PKE) measurements on the \(S\) layer side through the bilayer’s \(T_C\) using a Sagnac interferometer. The thickness of the \(S\) layer was fabricated to be larger than the optical skin depth in order to make sure that our experiment doesn’t pickup any magnetic moment from the \(F\) layer. \(\xi_s\) dependence of the effect is studied by comparing the results in \(Ni/Pb\) and \(Ni/Al\) samples.

\(^1\)Work supported by Center for Probing the Nanoscale, NSF NSEC Grant 0425897 and by DOE grant DEFG03-01ER45925

3:30PM D10.00004 Investigation of the role of Al/CoFe interface in proximity effect of Nb/Al/CoFe \(^1\), K. CHAR, JUNHYUNG KWON, WENJIAN LU, Seoul National University, MDPL TEAM — When a few nm-thick Al layer is inserted between Nb and ferromagnetic (F) layers such as CoFe, Ni, or CuNi, the superconducting critical temperature of the trilayers increases rapidly almost to a level of Nb/Al bilayers. In order to understand the role of Al/CoFe interface in the proximity effect of Nb/Al/CoFe, we have added Mg and Au scattering centers and found different behavior. The Mg scattering center did not change the critical temperature behavior of Nb/Al/CoFe, while the Au scattering centers reduced the critical temperature. The results point toward the importance of spin-orbit scattering. In addition, tunneling spectroscopy data on Nb/Al/F vs. on Nb/F will be presented in order to further characterize the role of Al/F interfaces.

3:42PM D10.00005 Magnetic property change by superconductivity in Py-Nb Hybrid system\(^1\), DAVID MURAKAMI, MICHAEL HETMAN, JIYEONG GU, Department of Physics and Astronomy, California State University, Long Beach — Recently ferromagnet/superconductor systems have attracted a great attention due to their scientific interest and potential for the technological application. So far, most of the work focused on the superconducting property change by magnetism in the hybrid system, and only few researches focused on the magnetic property change by superconductivity. In this presentation we will focus on the magnetic property change of the system by superconductivity when the system goes through the superconducting transition. We have investigated different types of hybrid structures including Py/Nb bilayer, multilayer, and composite systems. To separate out the signal from superconductor, we also measured the single Nb film. We measured the magnetization as a function of temperature and compared it between in a normal state and a superconducting state for the different types of structures. It showed strong magnetic history dependence.

\(^1\)This project is supported by Research Corporation Grant #CC6756 and NSF MRI Grant #0619909

3:54PM D10.00006 Proximity effect in MgB\(_2\)-Permalloy hybrid system\(^1\), APRIL O’BRIEN, JIYEONG GU, Department of Physics and Astronomy, California State University, Long Beach — Recently ferromagnet/superconductor systems have attracted a great attention due to their scientific interest and potential for the technological application. So far, most of the work has been done for Nb with ferromagnetic metals or high temperature oxide superconductors with magnetic oxides. In this presentation we will discuss the proximity effect in magnesium diboride (MgB\(_2\))/Py thin films, where the superconducting property changes due to the adjacent Py layer. Even though the good electronic properties such as large critical current density and large coherence length of MgB\(_2\) make it a good candidate for superconducting electronic applications, depositing a good-quality in-situ MgB\(_2\) thin film is still challenging. Especially for the multilayer deposition, it is ideal to deposit all the layers in-situ without ex-situ treatment. We used a sputtering to deposit the MgB\(_2\) layer in-situ and made a hybrid system with Py. We found that the substrate temperature during the MgB\(_2\) deposition is the most important parameter to determine the superconducting transition temperature of the sample. In addition to the proximity effect we will also discuss the problem with a sputtering method for MgB\(_2\) deposition.

\(^1\)This project is supported by Research Corporation Grant #CC6756 and NSF MRI Grant #0619909

4:06PM D10.00007 Spin-switch effect in Permalloy-Niobium hybrid system\(^1\), JIYEONG GU, MICHAEL HETMAN, Department of Physics and Astronomy, California State University, Long Beach — Proximity effect in ferromagnet (F)/superconductor (S) systems has become a center of attention recently. It has been well known that the superconducting property is modified when the magnetization of the adjacent F layer changes. Especially when the superconducting transition temperature changes as a function of the magnetization of the F layers, the system can work as a switching device. In this presentation we compare three different Py-Nb hybrid structures; Py/Nb bilayer, Py/Nb/Py/FeMn spin valve, and Nb/Py/Nb/Py/FeMn \((S-F-F)\) structure. We discuss the similarity and the difference in magnetic and transport properties of these three structures. When the Nb layer is thick in bilayer or \(S - F - F\) structure, the device showed a change between zero resistance (superconducting state) and finite resistance (normal state) by applying a small external magnetic field, where the shift in transition temperature is greater than the transition width, and this gave a large magnetoresistance effect \((|R(0)-R(H)|)/R(0)=\infty)\).

\(^1\)This project is supported by Research Corporation Grant #CC6756 and NSF MRI Grant #0619909

4:18PM D10.00008 Anomalous transport property in the single-crystal Co nanowire with superconducting electrodes\(^1\), JIAN WANG, NITESH KUMAR, MINGLIANG TIAN, QI ZHANG, JAINENDRA JAIN, THOMAS MALLOUK, MOSES H.W. CHAN, Center for Nanoscale Science, Penn State University — Transport measurements were made on individual single-crystal Co nanowire with four focused ion beam (FIB) deposited tungsten (W) electrodes, which are superconducting below 5 K. It was found that the 2 microns long Co nanowire shows a sharp and large resistance peak near the onset transition temperature \(T_C\) of W and a rapid resistance drop below \(T_C\). The large, 50% resistance drop at low temperature suggests the proximity effect from superconducting W electrodes extends to a large fraction of the ferromagnetic Co nanowire. The resistance peak is not seen in the Au nanowire with same superconducting W electrodes. Measurements on a Co nanowire contacted with FIB deposited non-superconducting Pt electrodes show no change in resistance.

\(^1\)Work supported by NSF MRSEC program under grant DMR-0213623.
4:30PM D10.00009 Transport properties of hybrid superconductor/ferromagnet nanowires fabricated by electrodeposition.\(^1\). NITESH KUMAR, JIAN WANG, QI ZHANG, MINGLIANG TIAN, MOSES H.W. CHAN, Center for Nanoscale Science, Penn State University — We have fabricated multilayer nanowires with alternating superconducting and ferromagnetic segments using template-based electrodeposition. Nanowires are fabricated with different diameters and length, with individual segments on the length scale of few hundreds of nm to few microns, using both porous polycarbonate and anodized alumina membranes. We have used Pb as the superconducting and Co or Ni as the ferromagnetic components. Structural characterizations done with X-ray diffraction and Transmission Electron Microscope demonstrated that Pb and Co segments are good single crystal whereas Ni segments are polycrystalline. We have done electrical transport measurements on arrays of multilayer nanowires (embedded inside the template) showing interesting magnetoresistance behaviors below the superconducting transition temperature of Pb. Four terminal electrical measurements on a single multilayer nanowire are in progress.

\(^1\)Work supported by NSF under a MRSEC grant, DMR-0213623.

4:42PM D10.00010 Ferromagnetic Josephson Resonance, IVANA PETKOVIC, MARCO APRILI. Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, UMR 8502, F-91405 Orsay Cedex, France — Ferromagnetic Josephson junctions with negative ($\pi$-) coupling behave as phase sources, a potentially very useful component of quantum electronics. In order to elaborate sophisticated circuits, it is crucial to understand the interplay between spin- and superconducting phase dynamics. For that purpose, we fabricated strongly underdamped sub-micron Josephson junctions. We measured the critical current at zero voltage as a function of the applied magnetic field. The finite magnetization in the junction induces a shift in the Fraunhofer pattern which is invariant under time reversal. For a voltage such that the Josephson frequency matches the ferromagnetic resonance, we observe a reduction of the critical current due to the absorption of the Josephson radiation by the ferromagnetic layer. We have investigated the effect of an external microwave radiation and of the magnetic field. The resonances appear as satellites at every Shapiro step and they are shifted in energy by the magnetic field as expected. The high sensitivity of the ac Josephson effect to a small amount of spins opens up new routes for ESR in nano-magnetism.

4:54PM D10.00011 Theory of spin wave excitation by Josephson current in a superconductor/ferromagnet/superconductor junction, SHIN-ICHI HIKINO, MICHIAYASU MORI, SABURO TAKAHASHI, SADAMICHI MAEKAWA, Institute for Materials Research, Tohoku University — The Joseph effect in a superconductor/ferromagnet/superconductor junction has been of considerable interest in recent years. Current-voltage (I-V) characteristics of superconducting weak links are studied by the resistively shunted junction (RSJ) model, which describes phase dynamics of superconductors (SC). The ferromagnet (F) has spin waves (SW). Therefore, in an S/F/S junction, it is important to treat the spin- and phase dynamics in an equal footing. However, the spin dynamics has not received much attention in the study of an S/F/S junction. We study the effect of the spin dynamics on the phase dynamics in an S/F/S junction. The RSJ model is extended to include the spin dynamics using gauge invariant phase difference between superconducting leads. We find that the I-V characteristics show step structures. The voltage at the steps is proportional to the SW energy in F. The origin of step structures will be discussed.

Monday, March 10, 2008 2:30PM - 5:18PM – Session D11 DCMP: Inhomogeneous Superconductors and Transport Morial Convention Center R09

2:30PM D11.00002 Disorder, Metal-Insulator crossover and Phase diagram in high-T\(_c\) cuprates, FLORENCE RULLIER-ALBENQUE, SPEC - CEA, HENRI ALLOUL, LPS - CNRS, FEDOR BALAKIREV, NHFML - Los Alamos, CYRIL PROUST, LNCMP - CNRS — We have studied the influence of disorder induced by electron irradiation on the normal state resistivities \(\rho(T)\) of optimally and underdoped YBa\(_2\)Cu\(_3\)O\(_y\) single crystals, using pulsed magnetic fields up to 60T to completely restore the normal state. We evidence that point defect disorder induces low \(T\) upturns of \(\rho(T)\) which saturate in some cases at low \(T\) in large applied fields as would be expected for a Kondo-like magnetic response. Moreover the magnitude of the upturns is related to the residual resistivity, that is to the concentration of defects and/or their nanoscale morphology. These upturns are found quantitatively, K. H. SARWA, B. TAN, KEVIN A. PARENDO, YEN-HSIANG LIN, Disorder-Tuned Superconductor-Insulator Transition, Department of Physics, University of Virginia — Highly disordered superconducting thin films exhibit a variety of novel phenomena, such as a possible metallic phase intervening the superconducting and the insulating state, and a huge peak in the magnetoresistance curve. Different theories have been proposed, including the quantum-vortex theory, the percolation picture of superconducting islands embedded in a normal metal, and the Bose metal theory. We propose that a drag resistance measurement in a bilayer setup would easily be able to determine which of the models applies. In such an experiment, two thin film superconductors are fabricated parallel to each other, separated by a thin insulator. A current bias is applied in one layer, and a voltage appears in the other due to the interaction between vortices (as in a Giaever transformer), or charge carriers (e.g., Coulomb drag), in different layers. Our calculation of the drag resistance in the various pictures will be discussed.

2:54PM D11.00003 Drag resistance in bilayer disordered superconducting thin films, YUE ZOU, ALLEN M. GOLDMAN, University of Minnesota, Minneapolis, MN 55455, USA — The effect of a perpendicular magnetic field on disordered, amorphous and insulating indium oxide thin films has been investigated. The temperature dependence of the resistance in zero magnetic field, the magnetoresistance pattern which is invariant under time reversal. For a voltage such that the Josephson frequency matches the ferromagnetic resonance, we observe a reduction of the critical current due to the absorption of the Josephson radiation by the ferromagnetic layer. We have investigated the effect of an external microwave radiation and of the magnetic field. The resonances appear as satellites at every Shapiro step and they are shifted in energy by the magnetic field as expected. The high sensitivity of the ac Josephson effect to a small amount of spins opens up new routes for ESR in nano-magnetism.

2:42PM D11.00010 Ferromagnetic Josephson Resonance, IVANA PETKOVIC, MARCO APRILI. Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, UMR 8502, F-91405 Orsay Cedex, France — Ferromagnetic Josephson junctions with negative ($\pi$-) coupling behave as phase sources, a potentially very useful component of quantum electronics. In order to elaborate sophisticated circuits, it is crucial to understand the interplay between spin- and superconducting phase dynamics. For that purpose, we fabricated strongly underdamped sub-micron Josephson junctions. We measured the critical current at zero voltage as a function of the applied magnetic field. The finite magnetization in the junction induces a shift in the Fraunhofer pattern which is invariant under time reversal. For a voltage such that the Josephson frequency matches the ferromagnetic resonance, we observe a reduction of the critical current due to the absorption of the Josephson radiation by the ferromagnetic layer. We have investigated the effect of an external microwave radiation and of the magnetic field. The resonances appear as satellites at every Shapiro step and they are shifted in energy by the magnetic field as expected. The high sensitivity of the ac Josephson effect to a small amount of spins opens up new routes for ESR in nano-magnetism.
3:06PM D11.00004 Granularity-induced field-hysteresis of transport critical current in patterned coated conductors, A. A. GAPUD, A. KHAN, University of South Alabama, D. K. CHRISTEN, F. A. LIST III, R. FEENSTRA, Oak Ridge National Laboratory — In superconducting coated conductors such as RABiTS and IBAD films, intergranular misorientations have been effectively minimized, but a small number of local, higher-angle misorientations remain. One important effect of such weak links is the hysteresis of the critical current density $J_c$ with respect to applied field $H$. Brought about when large circulating currents trapped within adjacent grains produce a focused field within the grain boundaries (GB’s) which can partially cancel out $H$ when applied field is decreasing, thus shifting the maximum $J_c$ from zero $H_{0}$ to a finite field where the local field at the GB is at minimum. This effect has been seen recently in measurements of magnetization (induced) currents, but has not been documented using transport (applied) current. However, in samples that are patterned into conduits 200 μm wide or less, the hysteretic effect on transport $J_c$ is clearly seen. This discrepancy between ‘magnetization $J_c$’ and ‘transport $J_c$’ may be due to differences in voltage criterion between the two types of measurement, as will be discussed. Systematic measurements and analyses will be presented, along with ramifications for applications.

1Research at ORNL sponsored by US Department of Energy

3:18PM D11.00005 Disorder induced resistivity upturns in metallic cuprates, BRIAN M. ANDERSEN, Nano-Science Center, Niels Bohr Institute, University of Copenhagen, WEI CHEN, PETER J. HIRSCHFELD, Department of Physics, University of Florida — We propose that experimentally observed resistivity upturn of cuprates at low temperature may be explained by properly accounting for the effects of disorder in a strongly correlated metallic host. Calculating DC transport using real space exact diagonalization of a Hubbard model treated in an inhomogeneous Hartree-Fock approximation, we find that correlations induce magnetization around impurities with screening length which increases strongly as temperature decreases, giving rise to additional magnetic scattering which causes the resistivity upturn. This paramagnetic response together with the electronic band structure effect is capable of explaining the magnetoresistance as observed in disordered optimally doped YBCO.

3:30PM D11.00006 Interrelations between superconducting properties and defect evolution in neutron irradiated YBa$_2$Cu$_3$O$_{7-x}$. VIOREL SANDU, GHEORGHE ALDICA, National Institute of Materials Physics, ELENA SANDU, National Institute of Nuclear Physics and Engineering “Horia Hulubei”, PETRU NITA, METAV-Research and Development Bucharest — We investigated the effect of neutron irradiation on the electric and magnetic properties, as well as the enhancement of the critical current density, of ceramic YBa$_2$Cu$_3$O$_{7-x}$ (LiF)$_x$ samples. The superconducting properties of the virgin samples reach the optimal values for $x = 0.04$. Up to the same $x$ value, the neutron irradiation up to $5 \times 10^{17}$ neutrons/cm$^2$ enhances the superconducting response (critical temperature, transition width, etc) and double up the magnetic irreversibility. For $x \geq 0.08$, all the superconducting properties are depressed whereas the increase of the irreversible magnetization is still present but less spectacular. The analysis of this behavior suggests a self-organization of the defects at low LiF content while for $x \geq 0.08$ they are uniformly distributed within sample.

1This work was supported by the National Authority for Science and Technology under the Project CEEX 45/2006

3:42PM D11.00007 Negative Nernst effect in simulations of granular superconductors, ANDREAS ANDERSSON, JACK LIDMAR, KTH Stockholm — The Nernst effect has recently become an important probe of superconducting fluctuations in high-Tc superconductors. The sign of the Nernst coefficient $\alpha$ is believed to be negative for metallic cuprates. Using real-space exact diagonalization, we find that $\alpha$ is negative for certain concentrations of dopants.

4:06PM D11.00009 Isotope Effect in High-Tc Superconductors, DALE HARSHMAN, Physikon Research Corp., JOHN DOW, Arizona State University, ANTHONY FIORY, New Jersey Institute of Technology — For high-Tc superconductors in which transition temperatures, $T_c$, are reduced by doping, the oxygen isotope effect (OIE) coefficient in $T_c$ is shown to increase systematically with the pairing-breaking rate and with the valence difference between the substituted and native ions. Moreover, the OIE tends to zero as one approaches optimum (or ideal) stoichiometry at which the quality of the superconducting condensate is maximized. In materials with isovalent substitutions, e.g., Sr for Ba or Zn for Cu in YBCO, the small OIE of the parent compound is magnified, owing to pair-breaking disorder. In materials with heterovalent substitutions, e.g., La or Pr for Ba, where carrier densities are necessarily changed, pair breaking induces a much larger OIE. A seminal case is Pr-doped YBCO, where the decrease in $T_c$ observed with Pr doping arises from pair-breaking caused by Pr-on-Ba-site defects. Without the defects, $T_c$ is invariant, providing strong evidence against phononic mechanisms. The fact that $T_c$ drops when Pr substitutes for Ba, but not for Y, indicates that the superconducting hole condensate resides in the BaO layers, where pair-breaking degrades $T_c$ and dramatically increases the OIE. Superconductive pairing modeled on Coulomb coupling between the hole and the electron layers is shown to resolve the shortcomings in electron-electron interactions.

4:18PM D11.00010 Rich Behavior of the Critical Currents of Magnetically-Doped Superconducting Films in Applied Magnetic Fields, JEFFREY Wasserman, NINA MARKOVIC, Johns Hopkins University — Films of MoGe were grown with varying dopant levels of cobalt contamination. Critical currents curves reveal significantly different behavior depending on the polarity of the current with respect to the applied field. At sufficiently-high dopant concentrations, the critical current increases with increasing magnetic field intensity for one polarity of current. We will discuss these results in terms of pair-breaking effects of magnetic fields and magnetic impurities.

1This work was supported in part by the National Science Foundation under grants DMR-0547834 and DMR-0520491 (MRSEC), and the Alfred P. Sloan Foundation under grant BR-4380, and ACS PRF # 42952-G10.
4:30PM D11.00011 Analytic description of the transport $J_\epsilon(B)$ dependence of HTS thin films in small magnetic fields. Jens Hännisch, Francesco Grilli, Los Alamos National Laboratory, Mail Stop T004, Los Alamos, 87545 NM, Sebastian Engel, Bernhard Holzapfel, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — Often, e.g. for deconvolution processes and field distribution calculations, an analytical function for the $J_\epsilon(B)$ dependence of high-$T_c$ thin films is needed. The parameters of these functions should still have a physical meaning regarding the intrinsic and extrinsic sample properties. Starting with the modified Kim model, described by Xu et al., we found an excellent function by introducing a sharpness parameter $\beta$. This parameter describes the shape of $J_\epsilon(B)$ between the low-field plateau (single vortex pinning regime) and the power-law dependence at higher fields. The temperature dependence of all fitting parameters will be discussed. Furthermore, the importance of the field dependence of the $\nu$ value for distinguishing different pinning regimes will be illustrated.

4:42PM D11.00012 Investigation of Vortex Pinning Anisotropy in the High Temperature Superconductor YBa$_2$Cu$_3$O$_{7-\delta}$, Andra Petrean-Troncalli, Austin College, Lisa Paulius, Western Michigan University, Heather Quantz, Austin College, Valentine Tobos, Lawrence Technological University, Wai-K Kwok, Argonne National Laboratory — Columnar defects have proven to be highly effective at pinning vortices, but most studies have been performed with the defects oriented either perpendicular or at large angles relative to the superconducting Cu-O planes. These studies have shown that the intrinsic pinning anisotropy of the crystal can actually be reversed by sufficiently strong columnar defects oriented parallel to the Cu-O planes. We have preliminary data that indicate that the pinning anisotropy is actually enhanced for columnar defects introduced parallel to the superconducting Cu-O planes. A single crystal of YBa$_2$Cu$_3$O$_{7-\delta}$ was polished down to a narrow width of 27 $\mu$m, allowing heavy ions to penetrate the crystal along the ab-plane. The crystal was irradiated with 1.4 GeV $^{208}$Pb ions to a dose matching field of 1T.

5:06PM D11.00014 Interface superconductivity in bi-layers of insulating and overdoped metallic La$_{2-x}$Sr$_x$CuO$_{4+\delta}$, Adrian Gozar, Gennady Logvenov, Anthony Bollinger, Ivan Bozovic, Brookhaven National Laboratory — We report on properties of thin superconducting (SC) sheets obtained in La$_{2-x}$Sr$_x$CuO$_{4+\delta}$ bi-layers of overdoped, non-superconducting (x = 0.45) and insulating (x = 0) films grown by molecular beam epitaxy. Superconductivity is confined to a thickness of $\approx$ 2 nm from the interface. The observed transition temperatures have values $T_c$ = 15 K, 30 K and 50 K depending on the layering sequence and oxidation state of the insulating material. Transport measurements are used to determine the screening properties of the quasi-2D SC sheets and the data in bi-layers are compared to results from single-phase films and bulk crystals.

Monday, March 10, 2008 2:30PM - 5:18PM – Session D12 DCMP: Theory of Ferroelectric, Multiferroic, and Other Structural Transitions Morial Convention Center 203

2:30PM D12.00001 Dynamics of domains switching in epitaxial BaTiO$_3$/SrTiO$_3$ superlattices from first principles. Sergey Lisenkov, Inna Ponomareva, Laurent Bellaiche, University of Arkansas — Superlattices (SL) consisting of alternating layers of perovskite oxides can possess properties that are dramatically different from those of bulk ferroelectrics. [BaTiO$_3$/SrTiO$_3$]$_n$ (BT/ST) SL with relatively large periods exhibit novel nanostripe domains for some specific epitaxial strains and within a particular temperature window [1]. Here, an effective Hamiltonian approach is used within molecular dynamics method to predict the evolution of these nanostripe domains in BT/ST SL under an ac electric field applied along the SL growth direction. For any investigated frequency, four different regimes occur, depending on the magnitude of the electric field. Region I that consists of nanostripe domains in both BT and ST layers; Region II that exhibits nanostripe domains in BT layers while possessing monodomains in ST layers; Region III where bubble domains in BT layers coexist with monodomains in ST layers; and Region IV where monodomains form in both BT and ST layers. The dependency of the domain velocities, activation and critical fields on the field frequency is revealed. [1] Lisenkov et al., Phys. Rev. B, 76, 020102(R) (2007).

2:42PM D12.00002 Ferromagnetic-like closure domains in ferroelectric ultrathin films: First principles simulation. Javier Junquera, Pablo Agudo-Puente, Dep. CITIMAC, Universitad de Cantabria, Avda. de los Castros s/n, E-39005, Santander, Spain — We simulate from first-principles the energetic, structural, and electronic properties of ferroelectric domains in ultrathin capacitors made of a few unit cells of BaTiO$_3$ between two metallic SrRuO$_3$ electrodes in short circuit. The domains are stabilized down to two unit cells, adopting the form of a domain of closure, common in ferromagnets but only recently detected experimentally in ferroelectric thin films. The domains are closed by the in-plane relaxation of the atoms in the first SrO layer of the electrode, that behaves more like SrO in highly polarizable SrTiO$_3$ than in metallic SrRuO$_3$. Even if small, these lateral displacements are essential to stabilize the domains, and might provide some hints to explain why some systems break into domains while others remain in a monodomain configuration. An analysis of the electrostatic potential reveals preferential points of pinning for charged defects at the ferroelectric-electrode interface, possibly playing a major role in films fatigue.

Supported by NSF grants DMR-0404335, DMR-0908054, DMR-0701558, by ONR grant N00014-04-1-0413, by DOE grant DE-FG02-05ER46188

Work supported by Spanish MEC under Projects FIS2006-02261 and FPU AP2006-02958

3Work supported by Spanish MEC under Projects FIS2006-02261 and FPU AP2006-02958
2:54PM D12.00003 The theory of domain patterns in ferroelastics, ALLAN JACOBS, Physics, University of Toronto — The theory of ferroelastic domain patterns is well developed and it explains qualitatively the domain patterns observed experimentally in many materials. It is known that much of the complexity of these patterns, which differ remarkably from those in conventional order-parameter systems, results from the differential rotation associated with domain walls. But there has been no direct confrontation between theory and experiment at a more quantitative level. I propose here such a confrontation. Specifically, I shall present predictions (obtained from numerical work) of the atomic displacements at the collision of orthogonal domain walls in tetragonal-orthorhombic ferroelastics and suggest that they be compared with HREM images of these materials.

3:06PM D12.00004 Peculiar ordering in flat ferroelectric nanoparticles driven by lattice misfit, IVAN NAUMOV, ALEX BRATKOVSKY, Hewlett-Packard Laboratories — Flat free-standing ferroelectric (FE) nanoparticles tend to have a vortex-like polarization ordering with the in-plane polarization that curls around an out-of-plane vortex core axis. The question is, if such a structure is still a ground state in presence of noticeable misfit strains induced by a substrate, and whether the 180° stripe domains may form, similarly to the case of ultra thin FE films? Here we perform an ab initio based study of disk- shaped Pb(Zr1−Ti1)O3 and BaTiO3 nanoparticles that have the vortex ground state when no stress is applied. Our study leads to the following findings for the disks having circular and square footprint: (i) under strong enough compressive strains the curling state is no longer stable and yields to a multi-domain structure with an out of-plane polarization, and different possible in-plane domains: triangle, stripe-like, or “bubble” states. (ii) each separate domain, regardless of its shape, runs through the entire thickness of a disk, and (iii) the 180° stripes occur only under special conditions depending on the shape and chemical composition of the nanostructures. Further, we discovered that starting with the vortex state and then increasing the compressive strains may lead to a metastable bi- or multi-domain phase different from the ground state obtained by gradual cooling at a fixed strain. This leads to a novel hysteretic behavior as a function of the misfit strain.

3:18PM D12.00005 Static and Dynamic Properties of Ferroelectric Nanostructures and Multiferroic Bulk Systems: A Multiscale Approach1, T. MICHAEL, S. TRIMPER, Martin-Luther-University, Halle, Germany, J.M. WESSELINOWA, University of Sofia, Bulgaria — Ferroelectric nanostructures and multiferroic bulk systems are studied in a multiscale approach. The excitation energy, associated damping of ferroelectric modes and polarization are presented as a function of temperature, defect concentration, size and shape. The softening of the mode is strongly influenced by the kind of doping ions, the surface configuration and the defect composition. The analysis is based on a modified Ising model in a transverse field. A Green’s function technique in real space provides the static and dynamic properties, which differ significantly from the bulk behavior. Additionally, a mesoscopic approach is carried out similar to the Landau-Lifshitz equation with Gilbert damping for ferromagnets. The temperature dependence of the damping parameters is discussed. The analysis is extended to multiferroic bulk systems, where the magnetic moments interact via the Heisenberg model and the multiferroic coupling term differs for hexagonal and orthorhombic materials. We present the dielectric function and the dynamic properties of the coupled model by applying previous methods.

1Supported by the International Max Planck Research School for Science and Technology of Nanostructures and the SFB 418.

3:30PM D12.00006 A new order parameter in complex dipolar structures, SERGEY PROSANDEEV, LAURENT BELLAICHE, University of Arkansas — Microscopic models have been used to reveal the existence of a new order parameter that is associated with many complex dipolar structures in magnets and ferroelectrics. This overlooked order parameter involves a double cross product of the local dipoles with their positions. It provides a measure of subtle microscopic features, such as the helicity of the two domains inherent to onion states, curvature of the dipolar pattern in flower states or characteristics of set of vortices with opposite chirality (e.g., distance between vortices’ centers and/or magnitude of their local dipoles). This work is mostly supported by DOE grant DE-FG02-05ER46188. We also acknowledge support from ONR grant N00014-04-1-0413 and NSF grants DMR-0701558, DMR-0404335 and DMR-0800504 (C-SPIN). Some computations were made possible thanks to the MRI Grants 0421099 and 0726252 from NSF.

3:42PM D12.00007 Microscopic origin of Magnetic Ferroelectrics in Non-collinear Multiferroics, CHEN FANG, JIANGPING HU, Purdue University — We propose a microscopic mechanism to understand the origin of magnetoelectric coupling in the best known multiferroic family RmOn (R =Tb, Dy...). The mechanism lies in the vanishing of electric current in an insulator. A spontaneous electric polarization is thus necessary, as it causes an electric current through a spin-orbit coupling to cancel another nonzero local electric current induced by a non-collinear modulated magnetic structure. Within this counter-balance mechanism, the magnitude of the ferroelectric order is determined by the magnetic order parameter and the spin-orbit coupling strength. Based on the theory, we predict a general physical limit for the value of ferroelectricity.

3:54PM D12.00008 A theory for the multiferroic compound LiCu2O2, TRINANJAN DATTA, Department of Chemistry and Physics, Augusta State University, CHEN FANG, JIANGPING HU, Department of Physics, Purdue University — We investigate the possible coupling between ferroelectricity and magnetic structure in the zig-zag spin chain compound LiCu2O2. Based on a group theory analysis, we construct a multi-order parameter phenomenological model and show that a coupling involving the inter-chain magnetic structures and ferroelectricity is necessary in order to understand the experimental results of Park et al. The model is able to account for the electric polarization flip through π/2 and explain the occurrence of an electric polarization parallel to an applied external magnetic field.

4:06PM D12.00009 Phase-field model of strain-induced grain-boundary premelting1, NAN WANG, ROBERT SPATSCHEK, ALAIN KARMA, Physics Dept and CIRCs, Northeastern University — Grain-boundary premelting depends in a complex way on the relative magnitude of the solid-liquid interfacial free-energy and grain boundary energy as well as temperature and strain. We study this dependence in a bicrystal geometry using a mesoscale phenomenological three-order parameter phase-field model. This model describes the short scale attractive or repulsive interaction between crystal-melt interfaces and macroscopic linear elasticity including the important effect of the density contrast between solid and liquid. The model exhibits a rich behavior characterized by single or multiple premelting transitions between dry or wet grain boundaries with different liquid layer thicknesses as a function of applied tensile stress. The results have important implications for the phenomenon of liquid metal embrittlement associated with the stress-driven penetration of nanometric liquid films along grain boundaries.

1This research was supported by DOE grant DE-FG02-07ER46400 and the DOE Computational Materials Science Network.

4:18PM D12.00010 Incorporation of plasticity into the Landau-Ginzburg theory of martensitic phase transformations, ROMAN GRÖGER, TURAB LOOKMAN, Los Alamos National Laboratory, Theoretical Division — The Landau-Ginzburg theory of martensitic phase transformations has been utilized to reproduce the evolution of elastic texture in defect-free materials undergoing structural phase transformations. Generalizations of this theory to phase transformations that are accompanied by significant plastic distortions (as in U76Nb) have been little studied. We propose a simple model that demonstrates how to incorporate plasticity into the Landau-Ginzburg theory. In the presence of topological defects such as dislocations, the usual Saint Venant compatibility constraint becomes an incompatibility constraint and this is represented by a tensor field γij. In our case, the components of γij are expressed as gradients of the components of the Nye tensor that represent the dislocation density. The presence of dislocations induces large internal stresses in certain regions of the material, and these act as initiation sites for plastic deformation. When the external loading is applied, dislocations moving from these regions cause strain hardening that is detectable in experimental uniaxial measurements. This model serves as a starting point for further development of the framework of three-dimensional rate-independent theory of plasticity within the Landau-Ginzburg formalism.
4:30PM D12.00011 Phonon Driven BCC to Orthorhombic Transformation in U-Nb Alloys, AVADH SAXENA, TURAB LOOKMAN, Los Alamos National Lab — The martensitic transformation in uranium alloys is of great strategic importance. We study the crystallography and model the well characterized BCC to orthorhombic phase transformation in the shape memory alloy U-Nb for low Nb concentrations. Our predictions are consistent with the experimentally observed relationship between the BCC and orthorhombic phases. We find that this temperature induced transformation is driven by a specific zone boundary phonon that couples to a particular shear mode. We also obtain a Landau free energy for this transformation. In addition, we compare our results with a similar shuffle based mechanism in a related martensitic alloy AuZn.

4:42PM D12.00012 First-Principles Study of the Jahn-Teller Distortion in the Ti$_{1-x}$V$_x$H$_2$ and Zr$_{1-x}$Nb$_x$H$_2$ Alloys, RAMIRO QUIJANO, ROMEO DE COSS, CINVESTAV-Unidad Merida, DAVID SINGH, Oak Ridge National Laboratory, USA — The transition metal dihydrides TiH$_2$ and ZrH$_2$ present the fluorite structure (CaF$_2$) at high temperature but undergoes a tetragonal distortion with $c/a<1$ at low temperature. Electronic band structure calculations have shown that TiH$_2$ and ZrH$_2$ in the cubic phase display a very flat band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. In order to understand the role of band filling in controlling the structural instability of the transition metal dihydrides, we have performed a first-principles total energy study of the Ti$_{1-x}$V$_x$H$_2$ and Zr$_{1-x}$Nb$_x$H$_2$ alloys. The calculations were performed using FP-LAPW method within the (DFT) and we use the GGA for exchange correlation functional energy. The critical concentration for which the Jahn-Teller effect is suppressed, was determined from the evolution of the tetragonal-cubic energy barrier. We discuss the electronic mechanism of the structural-instability, in terms of the band filling. From the obtained results we find that the tetragonal distortion in TiH$_2$ and ZrH$_2$ is not produced only by a Jahn-Teller Effect. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

4:54PM D12.00013 Density functional analysis of long range order, T.R.S. PRASANNA, IIT Bombay — A density functional analysis of order-disorder transitions in alloys shows that ordering energy is stored in superlattice wavevectors. Thermal vibrations play a key role and lower the transition temperature, T$_c$, to the experimental value (741 K) from the mean-field value (993 K) in the Bragg-Williams model for beta brass, $\beta$-CuZn. An isotope effect with 4 K difference in T$_c$ is predicted for $^{63}$Cu$^{64}$Zn and $^{65}$Cu$^{64}$Zn in a Modified Bragg-Williams model. The above conclusions are shown to be applicable in magnetic transitions as well. Theoretical analysis shows that thermal vibrations alter the exchange and total magnetic ordering energy. Every microscopic theory of magnetic and alloy phase transitions must satisfy the twin criteria that ordering energy is a) stored in superlattice wavevectors and b) a function of temperature due to thermal vibrations. An isotope effect is predicted to be a universal feature of alloy and magnetic phase transitions. The nuclear-nuclear energy term, $E_{nn}$, converges without artificial parameters if zero point vibrations are included unlike the Ewald sum technique.

5:06PM D12.00014 Ab-initio study of the structural and magnetic properties for the fcc Fe-Co alloy, FILIBERTO ORTIZ-CHI, Cinvestav Unidad Mérida, AARON AGUAYO, Universidad Autónoma de Yucatán, ROMEO DE COSS, CINVESTAV Unidad Mérida — We have studied the structural and magnetic properties of the fcc Fe-Co alloy by means of first-principles calculations. For modeling the alloy we have used the ab-initio self-consistent Virtual Crystal Approximation. The ground state properties was calculated with the Fixed Spin Moment methodology and the Full-Potential LAPW method. For the exchange-correlation potential we have used the Generalized Gradient Approximation. For ferromagnetic fcc-Fe we find an anti-invar behavior (ELS<AEHS) with the co-existence of two ferromagnetic states (metamagnetism). For the fcc-FeCo alloy we find a progressive evolution of the metamagnetism with the Co concentration. Using the calculated total-energy vs the lattice parameter and the Boltzmann distribution function, we have obtained the lattice parameter as function of the temperature, in order to determine the thermal expansion coefficient $\alpha$ as function of the Co-concentration. We find that Fe65Co35 show an invar behavior.

1 This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

Monday, March 10, 2008 2:30PM - 5:18PM — Session D13 DCOMP: Computational Methods: Strongly Correlated and Many Body Systems
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2:30PM D13.00001 Maximally-localized Wannier functions for GW quasiparticles, D.R. HAMANN, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Recent efforts carrying the GW many-body approximation to self-consistency have given improved electronic-structure results. However, one is left with self-energy operators only on the grid of $k$ points used for Brillouin-zone integration, unlike the case of DFT where the local self-consistent potential allows calculation of the band structure on arbitrary $k$ points (e.g., along symmetry lines). As maximally-localized Wannier functions (MLWF) provide a basis for a highly accurate approach to band interpolation, we have combined the WANNIER90 code for MLWF with the self-consistent GW capabilities of the ABINIT code to efficiently extend the GW grid calculation to a full band structure. MLWF also provide an intuitive picture of the orbital character and bonding of groups of bands, as well as a quantitatively accurate measure of electric polarization. Differences between quasiparticles MLWF and their LDA counterparts examined to date (Si and perovskite SrZrO$_3$) have proven small, but the visualization of many-body effects through MLWF remains an intriguing possibility. 1. F. Bruneval et al., Phys. Rev. B 74, 045102 (2006). 2. N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12 847 (1997). 3. M. van Schilfgaarde et al., Phys. Rev. Lett. 96, 226402 (2006).

2:42PM D13.00002 Ab initio calculation of the excited state properties of spiropyran, KIOUPAKIS, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — The photochromism of spiropyran/merocyanine molecules has been the subject of many experimental and theoretical studies. However, several questions remain open, in particular the excited state dynamics and the role of the triplet state. In this work, we use ab initio techniques based on Density Functional Theory and Green’s functions methods based on the GW approximation to the electron self energy and Bethe-Salpeter equations to study the ground and excited states of spiropyran/merocyanine for various geometries. Our results are compared with previous work. This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and TeraGrid resources provided by SDSC and Indiana University.

2:54PM D13.00003 All-electron GW calculation of vanadium dioxide, REI SAKUMA, TAKASHI MIYAKE, FERDI ARYASETIAWAN, JST-CREST, AIST — We present the results of the GW calculation of metallic and insulating vanadium dioxide using a full-potential LMTO basis set. Our calculations show that it is crucial to take into account both the frequency dependence and the off-diagonal elements of the self-energy. We find that the usual 1-shot GW scheme, where the frequency expansion of the self-energy is truncated in the first-order, yields a large error ($>0.1eV$) in quasiparticle energies due to the unsmoothness of the self-energy. In both phases, the dynamical correlation effect within RPA leads to a plasmon satellite which can be seen in the self-energy in quasiparticle energies due to the unsmoothness of the self-energy. In both phases, the dynamical correlation effect within RPA leads to a plasmon satellite which can be seen in the self-energy.
3:06PM D13.00004 GW-based \textit{ab initio} downfolding aiming at strongly correlated electron system\textsuperscript{1}, KAZUMA NAKAMURA, Dept. of Applied Physics, Univ. Tokyo, TAICHI KOSUGI, Dept. of Physics, Univ. Tokyo, YOSHIHIDE YOSHIMOTO, ISSP, Univ. Tokyo, RYOTARO ARITA, RIKEN, MASATOSHI IMADA, Dept. of Applied Physics and JST-CREST, Univ. Tokyo — Aiming at \textit{ab initio} description of real complex systems under effects of strong electron correlations, we develop a GW-based downfolding scheme formulated in the plane-wave basis set. Our method is successfully applied to organic conductors, the family of (BEDT-TTF)$_2$X. At the heart of our downfolding scheme lies utilizing the energy hierarchy of the system \cite{1}: The low-energy hierarchy near the Fermi level (\(\epsilon \pm 2\sim 3\) eV) determines physics while is affected by the remaining high-energy part of hierarchy. We renormalize the high-energy part into low energy, based on the GW scheme. The renormalization generates a low-energy model characterized by renormalized transfers and effective screened Coulomb/exchange interactions, having frequency dependence arising from retarded screening by eliminated high-energy electrons. Thus, the low-energy frequency-dependent effective model is mapped out from the whole high- plus low-energy system in an \textit{ab initio} procedure. \cite{1} F. Aryasetiawan et al., Phys. Rev. B \textbf{70}, 19514 (2004); I. V. Solovyev and M. Imada, \textit{ibid.} \textbf{71}, 045103 (2005).

\textsuperscript{1}This work is supported by MEXT (Grant No. 17064004).

3:18PM D13.00005 GW Study of Actinides: \(\alpha\)-Uranium and \(\delta\)-Plutonium, R.C. ALBERS, A.N. CHANTIS, Los Alamos National Laboratory, M. VAN SCHILFGAARDE, Arizona State University, T. KOTANI, Arizona State University — We have applied the recently developed Quasiparticle Self-Consistent GW (QSGW) method to \(\alpha\)-U and \(\delta\)-Pu. This is the first time that the f-orbital electron-electron interactions in actinides have been treated by a first-principles method that goes beyond the level of the generalized gradient approximation. We show that the QSGW approximation for \(\alpha\)-U predicts a significant f-band narrowing when compared to GGA band-structure results. However, because of the low f-electron occupation number in U, ground-state properties are not significantly affected. This provides the first formal justification for the success of the LDA and GGA calculations in describing the ground-state properties of this material. For Pu we find that QSGW, like conventional band-structure calculations, predicts a static magnetic ground-state in contradiction with experiment. A non-magnetic solution is also presented. For \(\delta\)-Pu we show that the QSGW approximation predicts even stronger band narrowing than for U. Because of this and a larger f-occupation, the ground state properties are affected much more significantly than for U. Overall, because of its better treatment of correlation, we suggest that the QSGW solution rather than GGA should be a better starting point for future Dynamical Mean Field Theory (DMFT) and other correlation methods.

3:30PM D13.00006 The formation of stripes and the pairing of charge carriers in anisotropic materials\textsuperscript{1}, K.J.E. VOS, C. POVEY, J.M. TIPPER, University of Lethbridge — We have examined the formation of stripes and pairing in the anisotropic t - J model. We have used exact diagonalization methods on several different cluster sizes to examine the underdoped region. Evidence of unidirectional stripe formation in the charge and spin correlations was found. We have determined that the formation of stripes parallel to the Cu-O-Cu bonds enhances pairing and in the bulk limit there is a finite range of doping concentration where hole pairs will form. As the material becomes more anisotropic there is a phase transition that destroys the stripe. These results are consistent with the experimental data.

\textsuperscript{1}The computational infrastructure was provided by Westgrid. This work is supported by NSERC of Canada.

3:42PM D13.00007 Theory of the Normal State of the Copper-Oxide Superconductors\textsuperscript{1}, TING PONG CHOI, ROBERT G. LEIGH, PHILIP PHILLIPS, University of Illinois at Urbana Champaign — We show here that many of the normal state properties of the cuprates are consequences of the new charge 2e boson which we have recently (Phys. Rev. Lett. \textbf{99}, 46404 (2007) and arXiv:0707.1554) shown to exist in the exact low-energy theory of a doped Mott insulator. In particular, the 1) mid-infrared band, 2) the \(T^2\) contribution to the thermal conductivity, 3) the pseudogap, 4) the bifurcation of the electron spectrum below the chemical potential as recently seen in angle-resolved photoemission, 5) insulating behaviour away from half-filling, 6) the high and low-energy kinks in the electron dispersion and 7) T-linear conductivity all derive from the charge 2e boson. We also calculate the inverse dielectric function and show that it possesses two dispersing particle-hole branches as a function of momentum in the lightly doped regime. The second of the two branches is mediated by a new charge e composite excitation formed from the charge 2e boson and represents a distinctly new prediction of this theory. We propose that electron energy loss spectroscopy at finite momentum and frequency can be used to probe the existence of the second particle-hole branch.

\textsuperscript{1}We thank the NSF DMR-0605769 for partial support. This research was also supported in part by the NSF PHY05-51164.

3:54PM D13.00008 Imaginary-time formulation for strongly correlated transport in steady-state nonequilibrium\textsuperscript{1}, JONG E. HAN, RYAN J. HEARY, SUNY at Buffalo — We formulate steady-state nonequilibrium from the scattering state theory and show that an imaginary-time formalism exists for strongly correlated transport calculations in quantum dot devices\textsuperscript{2}. Equilibrium imaginary-time method is extended to the steady-state nonequilibrium by mapping the chemical potential difference in the quantum dot device into complex Matsubara voltage. Due to this formal similarity between equilibrium/nonequilibrium theories, we readily apply an equilibrium numerical technique to calculate the strong correlation effects in nonequilibrium. We use quantum Monte Carlo method to calculate Green functions at each Matsubara voltage and, after a numerical analytic continuation, we obtain nonperturbative Green function far from equilibrium. We show numerical results for the evolution of Kondo anomaly as a function of finite bias. We also discuss the splitting of Kondo anomaly at finite magnetic fields.

\textsuperscript{1}Supported by NSF DMR-0426826.


4:06PM D13.00009 Electron fractionalization and statistics of holons in doped quantum dimer models\textsuperscript{1}, DIDIER POILBLANC, Laboratoire de Physique Théorique, CNRS & Universite de Toulouse (France) — I introduce a doped two-dimensional quantum dimer model describing a doped Mott insulator and retaining the original Fermi statistics \cite{1}. This model shows a rich phase diagram including a d-wave hole-pair superconductor breaking translation symmetry (supersolid) at small doping, a bosonic superfluid at large doping and an exotic intermediate phase in-between. The hole kinetic energy is shown to favor binding of topological defects to the fermionic holons turning them into bosons, in agreement with arguments based on RVB wave-functions. Results are discussed in the context of cuprates superconductors and compared with those of a related bosonic doped quantum dimer model \cite{2}. \cite{1} D. Poilblanc, arXiv:0711.2229. \cite{2} A. Ralko, F. Mila, and D. Poilblanc, Phys. Rev. Lett. \textbf{99}, 127202 (2007).

\textsuperscript{1}Support from the French National Research Agency (ANR) acknowledged.
4:18PM D13.00010 Improvement on the STLS Approach and its Application to the Spin Fully-Polarized Low-Density Electron Gas, YASUTAMI TAKADA, ISSP, Univ. of Tokyo, KANAKO YOSHIZAWA, Dept. of Physics, Sophia Univ. — Four decades ago, Singwi, Tosi, Land, and Sjölander (STLS) proposed a theory that treats the local-field factor $C(q)$ and the static structure factor $S(q)$ in a self-consistent fashion. Because of its simplicity in practical calculations and reasonably good results for the correlation energy, this STLS framework has been recognized as a powerful theoretical tool to study short-range correlation beyond the RPA. At the same time, however, it has been realized that the STLS scheme has several shortcomings; among others, it does not satisfy the Pauli principle as exemplified by the fact that the on-top parallel-spin pair distribution function $g_{11}(0)$ becomes negative. In view of this situation, we propose an improved STLS approach in which a special procedure is added to the original STLS framework in order to impose the Pauli principle. This new scheme is successfully applied to the spin-fully polarized electron gas with the electron density parameter $r_s$ ranging from 1 to 100 to find that the correlation energy obtained by quantum Monte Carlo simulations is reproduced very accurately, along with satisfying $g_{11}(0) = 0$ and the non-negativity condition $g_{11}(r) \geq 0$. Implications of our results will be given in the context of the contribution to the density functional theory as well as to the spin structure of the Wigner-lattice state.

4:30PM D13.00011 Role of phonons and of finite temperature on the spectral function of a single hole in a quantum antiferromagnet, SATYAKI KAR, Department of Physics, Florida State University, Tallahassee, FL, 32306-4350, EFSTATIOS MANOUSAKIS, Department of Physics and MARTECH, Florida State University, Tallahassee, FL, 32306, and Department of Physics, University of Athens, Greece — Thermal broadening as well as the role of optical phonons are studied for a single-hole in a quantum antiferromagnet within the t-J (and the t-t'-t''-J) model. The non-crossing approximation (NCA) as well as the effect of vertex corrections (up to second order) are used to describe the coupling to spin waves and phonons up to intermediate range of coupling. Phonons at finite temperature are seen to broaden the quasiparticle peak and the string excitations are found to survive up to an intermediate phonon-coupling regime beyond which the NCA is expected to break down. The qualitative features of our results compare reasonable well with the recent high resolution angular resolved photoelectron spectroscopy.

4:42PM D13.00012 The Green’s Function of the 1D Breathing-Mode Polaron, GLEN GOODVIN, MONA BERCIU, University of British Columbia — We apply the Momentum Average approximations MA(0) and MA(1) to study the properties of the one-dimensional breathing-mode polaron. The results are analytical, numerically trivial to evaluate, exact for both zero bandwidth and for zero electron-phonon coupling, and are accurate everywhere in parameter space. Comparison with recent numerical data confirms this accuracy. We also show that by applying MA as a variational method with a suitably chosen enlarged subspace, we can obtain extremely high accuracy for both ground state and higher energy state properties. With only a slight increase in computational effort this allows us to obtain ground state and momentum-dependent results well within 0.1% error of the exact numerical data currently available. Although this work specifically looks at the breathing-mode model, we demonstrate that MA is applicable to all momentum dependent electron-phonon coupling models, and its accuracy can always be improved by systematically improving the approximation itself or by working in an enlarged variational subspace.

5:06PM D13.00014 Extensions of the Momentum Average approximation, MONA BERCIU, LUCIAN COVACI, University of British Columbia — We consider a well studied problem, the formation of polaron. Even for the simplest electron-phonon interaction (the Holstein model), an exact solution is only known in the asymptotic limits of zero coupling or zero free-electron bandwidth. A simple analytical approximation that turns out to be accurate for all coupling strengths (the Momentum Average approximation) has only been found recently. We discuss the extension of this method to various other situations in which polaron physics might be important. We show how the Momentum Average approximation can be used in answering questions regarding coupling of electrons to multiple phonon branches, formation of polarons in the presence of magnetic fields and the existence of multiple electron bands.

Monday, March 10, 2008 2:30PM - 5:30PM — Session D14 DAMOP GQI: Quantum Information Science in AMO — Morial Convention Center 205

2:30PM D14.00001 Quantum Information Aspects of Cold Fermi Systems, RAZVAN TEOODORESCU, Los Alamos National Laboratory — In the limit of fast switching of Feshbach resonance in cold fermionic systems, the dynamics is dominated by non-linear, coherent, multi-frequency quantum oscillations of the order parameter. This theoretical model is very rich and has known connections to several quantum field theories. In this talk, I will analyze the problem from the point of view of quantum information theory and indicate possible practical applications of the fast-switching regime.

2:42PM D14.00002 Coherent Control of Trapped Bosons, ANALABHA ROY, Graduate Student, University of Texas at Austin, LINDA REICHL, Director CQS — We investigate the quantum behavior of a mesoscopic two-boson system produced by number-squeezing ultracold gases of alkali metal atoms. The quantum Poincare maps of the wavefunctions are affected by chaos in those regions of the phase space where the classical dynamics produces features that are comparable to $\hbar$. We also investigate the possibility for quantum control in the dynamics of excitations in these systems. Controlled excitations are mediated by pulsed signals that cause Stimulated Raman Adiabatic passage (STIRAP) from the ground state to a state of higher energy. The dynamics of this transition is affected by chaos caused by the pulses in certain regions of the phase space. A transition to chaos can thus provide a method of controlling STIRAP.

The authors wish to thank the Robert A. Welch Foundation (Grant No. F-1051) for support of this work.
Phase transitions, entanglement and quantum noise interferometry in cold atoms. FLORIAN MINTERT, University of Freiburg. INDUBALA SATIJA, George Mason University. ANA MARIA REY, ITAMP. CHARLES CLARK, NIST. — Quantum entanglement represents one of the most fascinating features of quantum theory and has emerged as an important resource in quantum information science. Recent studies have suggested that the long range correlations that are established close to a quantum phase transition manifest themselves in a pronounced increase of entanglement. However, to show that is not an easy task given the fact that currently there is not consensus about the best method to define an entanglement measure for multi-particle systems. Using an entanglement measure that includes up to four point correlation functions we study the scaling properties of multi-particle entanglement in a one dimensional Ising chain around and at the critical point. Our study reveals that multiparticle entanglement indeed peaks at the phase transition, whereas pure biparticle entanglement measures often fail to reveal this feature. We discuss the connection between multiparticle entanglement measurements with noise correlations and the possibility of using these experimentally accessible quantities as a probe of entanglement in cold atomic systems.

Mapping phononic entanglement into and out of a quantum memory. HUI DENG, KYUNG S. CHOI, JULIEN LAURAT, H. JEFF KIMBLE, California Institute of Technology. — Recent developments of quantum information science critically rely on entanglement. In particular, scalable quantum networks require capabilities to create, store, and distribute entanglement among distant nodes via photon channels. Atomic ensembles can serve as such nodes. In the photon counting regime, heralded entanglement between atomic ensembles has been demonstrated via probabilistic protocols. However, an inherent drawback of such protocols is the compromise between the fidelity of entanglement and its preparation probability, which hinders the schemes’ scalability. Here we present a protocol where entanglement between atomic ensembles is created by coherent mapping of phononic entanglement. By splitting a single-photon and subsequent state transfer, we separate the generation of entanglement and its storage, enabling efficient scaling for high-fidelity quantum communication. After a programmable delay, chosen at 1ns, the stored entanglement is mapped back into photon modes with an overall efficiency of 17%. With improved retrieval efficiency and memory time, along with the development of on-demand single photon sources, our protocol enables the deterministic generation, storage, and distribution of entanglement among remote quantum memories for scalable quantum networks.

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Broadband Multi-Spot Optical Beam Steering with Independent 2D Addressability for Quantum Information Processing. CALEB KNOERNSCHILD, CHANGSOON KIM, Duke Univ. FELIX LU, Duke Univ. and Applied Quantum Tech., JUNGSANG KIM, Duke Univ. — While quantum computation utilizing trapped ions or neutral atoms has seen significant advances in recent years, the necessary scalability of such implementations is limited in part by the distribution of laser resources. The capability to address multiple qubit locations with a single laser is an essential element in moving these experiments beyond individual quantum gate demonstrations. An optical system utilizing micro-electromechanical system (MEMS) technology can provide a scalable solution to address a qubit array with multiple independent beams concurrently. Broadband coatings can accommodate a large range of wavelengths, while fabrication techniques allow expansion to multiple parallel laser beams over a large number of trap locations. We demonstrate a two-spot beam steering system using MEMS mirrors that can simultaneously and independently illuminate any of 25 different locations within a 5x5 array with 2 laser beams of different wavelengths. Mirrors with setting times of < 5µs have been fabricated allowing fast access times between qubits. Such systems can be used to implement two-qubit gates in a 1D or 2D array of qubits.

Toward a Wire-mediated Coupling of Trapped Ions. ROBERT CLARK, Institut für Quantenoptik und Quanteninformation, Innsbruck, Austria and Massachusetts Institute of Technology, Cambridge, MA, TONY LEE, NIKOS DANIILIDIS, SANKARANARAYANAN S., HARTMUT HÄFFNER, Institut für Quantenoptik und Quanteninformation, Innsbruck, Austria. — Most schemes for ion trap quantum computation rely upon the exchange of information between ion-qubits in the same trap region, mediated by their shared vibrational mode. An alternative way to achieve this coupling is via the image charges induced in a conducting wire that connects different traps. This was shown to be theoretically possible by Heinzen and Wineland in 1990, but some important practical questions have remained unaddressed. Among these are how the presence of such a wire modifies the motional frequencies and heating rates of trapped ions. We thus have realized this system as a 1 mm-scale planar segmented rf ion trap combined with an electrically floating gold wire of 25 microns diameter and length 1 cm. This wire is placed close to trapped ions using a set of piezoelectric nanopositioners. We present here experimental measurements of the motional frequencies and heating rates of a single trapped calcium ion as the wire is moved from 3.0 mm to 0.2 mm away from the ion. We discuss the implications of these results for achieving wire-mediated coupling in the present apparatus, as well as in future improved setups.
In our experiment, we measure the heating rate out of the motional ground state of a single Sr ion in a closed-cycle 4 K ion trap. The rich internal structure of polar molecular ions makes them attractive for interfacing with solid state systems in quantum information processing, yet it is this structure that makes trapping and detecting molecules difficult. We present an approach to this challenge which allows a superconducting cavity to be used as an integral part of a surface electrode ion trap, based on a closed-cycle cryostat operated at 4 K, and addressing the problem of molecule formation and detecting their presence. A mixture of Sr and SrCl ions is loaded into the trap by laser ablation. Subsequent laser cooling of the Sr ions sympathetically cools the molecular ions, producing a two-component Wigner crystal. This allows detection of the molecules using mass spectroscopy, observed indirectly through imaging of the Sr ions, or through coupling to microwave lines in the trap. Using a closed-cycle cryostat enables rapid testing and evaluation of ablation targets and trap geometries, at the cost of some trap vibration, measured to be below 100 nm in amplitude.

4:20PM D14.00012 Cavity cooling of $^{88}$Sr$^+$. DAVID LEIBRANDB, YAT SHAN AU, ISAAC CHUANG, MIT — Cavity cooling is a method of laser cooling which uses coherent scattering to cool atoms [V. Vuletić and S. Chu, PRL 84, 3787 (2000)]. The closed atomic transition used in Doppler cooling is replaced by a cavity resonance, so cavity cooling can be used to cool to sub-Doppler temperatures and is in principle applicable to complicated atoms or molecules without closed transitions. We describe an experiment to study three-dimensional cavity cooling of a single $^{88}$Sr$^+$ ion confined in a linear RF Paul trap. Large cooling rates can be attained by operating near the 422 nm $S_{1/2} \rightarrow F_{1/2}$ optical dipole transition and using a 5 cm long near-confocal Fabry-Pérot cavity with commercially available mirrors of finesse $10^4$. Given a cavity alignment error $\leq 10$ μm and a trap frequency of 1 MHz, the resolved sideband cavity cooling limit is $\leq 5$ motional quanta. We present details of the experimental proposal and its implementation.

4:44PM D14.00013 Microfabrication of Surface Electrode Ion Traps for Quantum Information Experiments. YUEFEI GE, SHANNON WANG, ISAAC CHUANG, MIT — Surface electrode ion traps, while promising for large-scale quantum computation, have long been challenged by ion heating rates which increase rapidly as trap length scales are reduced. Through a series of measurements on over fifteen traps, we show that ion heating rates are surprisingly sensitive to electrode material and morphology, and in particular, to details of the fabrication procedure. For example, one 75 μm size trap, made of chemically etched silver on a single crystal quartz substrate, showed a minimum heating rate of $\sim 40$ quanta/second, when prepared by annealing at 700°C in vacuum for one hour. This annealing smooths sharp edges, and significantly reduces breakdown voltage. However, if the annealing temperature is lowered to 720°C, leaving the breakdown voltage still robustly high, the heating rate jumps to $\sim 1000$ quanta/second. With electroplated gold, on a silver seed layer, a record low heating rate of $\leq 2$ quanta/second is obtained. We present details of the fabrication procedures, evaluate alternative electrode materials such as niobium nitride, and explain how these measurements were obtained with an ion trap operated at 6 Kelvin, containing a single strontium ion, sideway cooled to its quantum ground state of motion.

5:06PM D14.00014 Temperature dependence of decoherence in ion traps. YUEFEI GE, SHANNON X. WANG, ISAAC CHUANG, Center for Ultracold Atoms, MIT — Dense arrays of trapped ions provide one way of scaling up ion trap quantum information processing. However, miniaturization of ion traps is currently limited by sharply increasing motional state decoherence at sub-100 μm ion-electrode distances. This decoherence has been demonstrated to be thermally driven, providing a plausible route to reduce it. In our experiment, we measure the heating rate out of the motional ground state of a single Sr$^+$ ion in a cryogenic surface electrode ion trap. We present our results on the temperature dependence of the heating rates as a function of electrode temperature in 10-100 K range. Heating rates at 6 K are observed to be as low as two quanta per second, but increase rapidly with temperature.

5:18PM D14.00015 Individual ion addressing using a magnetic field gradient in a surface-electrode ion trap. SHANNON WANG, ISAAC CHUANG, YUEFEI GE, MIT — The ability to address individual ions is an important issue in using multiple trapped ions to perform quantum operations. Previous efforts have included using precisely focused laser beams aimed at only one ion at a time, which poses a significant technical challenge. An alternative is to use field-dependent transitions and a magnetic field gradient to shift the transition frequencies of ions as a function of position. This requires good stability of the local field in order to achieve desired fidelity of quantum operations. In a cryogenic Sr$^+$ ion trap we use the $5S_{1/2} \rightarrow 4D_{5/2}$ transition as an optical qubit, which can be Zeeman shifted using a bias field generated by external coils. We present a scheme to create a local field gradient by integrating current sources onto a microfabricated surface-electrode trap. Taking advantage of the cryogenic environment, we stabilize the field at the trap site using superconducting rings as flux shields. The rings can be integrated with the trap, simplifying implementation and improving alignment to the ions.

Monday, March 10, 2008 2:30PM - 5:18PM — Session D15 GQL: Focus Session: Foundations of Quantum Theory I — Morial Convention Center 207

2:30PM D15.00001 LeRoy Apker Award Talk: Testing Hidden-Variable Theorems with Single-Photon Entangled States. BRYCE GADWAY, SUNY Stony Brook / Colgate University — An ensemble of single photons created in a hyperentangled Bell state were used to test a broad class of Hidden-Variable Theorems (HVTs). Specifically, the class of HVTs based on the joint assumption of Realism and Non-Contextuality (NC) – the premise that values associated with one observable are independent of which commuting observables may be measured simultaneously – known as NCHVTs, and first examined by Bell as Kochen and Specker, uses these single-photon states entangled in polarization and direction of momentum. A Clauser-Horne-Shimony-Holt (CHSH) Inequality was applied, with the factorization condition that is usually satisfied by a Non-Locality assumption being instead satisfied by the assumption of NC, due to the inherently local nature of detection events for single particles. The basis rotations and projections necessary for testing the CHSH Inequality were accomplished using interferometers and standard polarization optical elements. A violation of the CHSH Inequality was observed, ruling out either Realism or Non-Contextuality – or possibly both. The tenability of Contextual HVTs remains, trivially, as the predictions of such a theory can map one-to-one to the predictions of Quantum Mechanics.
3:06PM D15.00002 Weak values and the Leggett-Garg inequality in solid-state qubits, ANDREW JORDAN, University of Rochester — The seminal paper of Aharonov, Albert, and Vaidman introduces the concept of a weak value as a statistical average over realizations of a weak measurement, where the system is both pre- and post-selected. By taking restricted averages, weak values can exceed the range of eigenvalues associated with the observable in question. We discuss how to implement a weak values measurement with solid-state qubits. In parallel activity, Leggett and Garg have devised a test of quantum mechanics for a single system using different ensembles of (projective) measurements at different times and correlation functions of those outcomes. The original motivation was to test if there was a size scale where quantum mechanics would break down. Introduced as a "Bell-inequality in time", the assumptions of macrorealism that could be verified by a non-invasive detector imply that their correlation function obeys a Leggett-Garg inequality that quantum mechanics would violate, formally similar to the inequality of Bell. We demonstrate that the proper notion of a classical weak value also demands these assumptions, and that furthermore a weak value can be non-classical if and only if a Leggett-Garg inequality can also be violated. We will discuss generalized weak values, where post-selection occurs on a range of weak measurement results. Our analysis is presented in terms of kicked quantum nondemolition measurements on a quantum double-dot charge qubit.

3:42PM D15.00003 Negative probabilities and measurement disturbance, LARS M. JOHANSEN, Buskerud University College — Feynman once said that "the only difference between a probabilistic classical world and the equations of the quantum world is that somehow or other it appears as if the probabilities would have to go negative". But what is the essential reason for probabilities going negative? Here it is demonstrated that negative probabilities are a direct consequence of measurement disturbance. The Margenau-Hill distribution, a quasiprobability taking negative values, is expressed in terms of the joint probability obtained in the successive measurement of two projectors. The quasiprobability takes negative values only if the measurement on the second projector is a weak measurement. We show that error-free which-path measurements are possible in this model that do not destroy the fringe visibility. On the other hand, does not require one to measure the fringe visibility. We show that neither the conventional uncertainty principle nor the recently-derived universal uncertainty principle place any restriction on the minimum root-mean-square momentum disturbance, once it is recognized that the which-path determination does not affect the measurement value of x, but only the appropriate two-valued function of x. We then develop a description of the problem in terms of only two-valued variables, and consider a completely general measurement model, which allows us to distinguish between the measurement error and what we call the "preparation error." We show that error-free weak measurement is only possible if the fringe visibility does not destroy the fringe visibility. On the other hand, we also show that there is a general tradeoff relation between preparational error and fringe visibility, which, for measurements obeying the "non-destruction" condition, reduces to Englert's inequality.

3:54PM D15.00004 The meaning of negative weak values, JAMES TROUPE, JEFF TOLLAKSEN, George Mason University — A number of approaches to quantum mechanics incorporate negative values for quantities that were classically positive, such as the Wigner-Moyal density approach or the Feynman negative probability approach, etc. In the re-formulation of quantum mechanics using weak values and weak measurements, we encounter a new situation where weak values of projection operators turn out to be negative. We emphasize the differences between these negative weak values and the negative values encountered in the other formalisms: in the previous formalisms, the mathematical entity whose average yielded the negative values are not density operators. While they do yield the correct average of a function, they also have non-physical aspects, i.e. mathematical artifacts, when the densities become negative. The reason is that if we attempt to actually measure such "negative" properties, then the result does not correspond to a physical observable in Hilbert Space. E.g. if we did attempt to cheat quantum mechanics by projecting onto p and x as densities simultaneously in Wigner-Moyal, then we obtain the parity operator, the most non-local result. On the other hand, in the case of weak values, we obtain a new situation: when we use a bonafide measuring device to measure these properties ideally, then the very same measuring device will yield the predicted negative weak values when the measurement interaction is simply weakened.

4:06PM D15.00005 Frame representations of quantum mechanics and the necessity of negativity in quasi-probability representations, CHRISTOPHER FERRIE, JOSEPH EMERSON, University of Waterloo — Several finite dimensional quasi-probability representations of quantum states have been proposed to study various problems in quantum information theory and quantum foundations. These representations are often defined only on restricted dimensions and their physical significance in contexts such as drawing quantum-classical comparisons is limited by the non-uniqueness of the particular representation. Here we show how the mathematical theory of frames provides a unified formalism which accommodates all known quasi-probability representations of finite dimensional quantum systems. Moreover, we show that any quasi-probability representation satisfying two reasonable properties is equivalent to a frame representation and then prove that any such representation of quantum mechanics must exhibit either negativity or a deformed probability calculus.

4:18PM D15.00006 Towards Testing Quantum Mechanics with Micro-Optomechanical Systems, DUSTIN KLECKNER, SUSANNA THON, University of California - Santa Barbara, EVAN JEFFREY, University of Leiden, DIRK BÖUWMEESTER, University of California - Santa Barbara and University of Leiden — We review our work in micro-optomechanical systems. Motivation for work on these systems is based in proposals to test quantum mechanics in new regimes. Although extremely challenging, creating a quantum superposition of a micro-optomechanical oscillator coupled to an optical cavity seems experimentally feasible with current technology. Additionally, the optomechanical systems used for this type of research have other applications, such as optical cooling, as recently demonstrated by several independent groups. We will briefly discuss the direction of our research in the near future, including the use of conventional cryogenics to cool the resonator and the prospects for several related types of devices.

4:30PM D15.00007 Decoherence and the Uncertainty Principle, DAVID CRAIG, Le Moyne College — The uncertainty principle is normally understood as representing a limit on the fundamental accuracy of simultaneous measurements of incompatible observables. In the context of consistent/decoherent histories formulations of quantum theory, we show that it may also be understood as quantifying the degree of course-graining necessary in order for histories of a quantum system to decohere. This follows as a consequence of a new inequality bounding the interference between histories in a consistent histories formulation of quantum theory.

4:42PM D15.00008 Noncontextuality and the Kochen-Specker Theorem, BRIAN LA COUR, University of Texas at Austin — The question of noncontextuality in a simple, two-qubit system is considered. It is shown that quantum theory is consistent with a noncontextual hidden variable interpretation, contrary to the conclusions of the Kochen-Specker theorem. The key to the proof is the recognition of a subtle but fundamentally important assumption regarding the dependence of the hidden variable probability distribution on the particular set of mutually commensurable observables chosen for measurement. Recent experiments to test noncontextuality will be discussed and their results reconciled with a hidden variable interpretation.

4:54PM D15.00009 Path detection and interference tradeoff in the double-slit experiment, JULIO GEA-BANACLOCHE, University of Arkansas, MASANAO OZAWA, Tohoku University, Japan — We study how the acquisition of "which-path" information leads to a loss of contrast in the double-slit interference setup. We show that neither the conventional uncertainty principle nor the recently-derived universal uncertainty principle place any restriction on the minimum root-mean-square momentum disturbance, once it is recognized that the which-path determination does not require one to measure x, but only an appropriate two-valued function of x. We then develop a description of the problem in terms of only two-valued variables, and consider a completely general measurement model, which allows us to distinguish between the measurement error and what we call the "preparation error." We show that error-free which-path measurements are possible in this model that do not destroy the fringe visibility. On the other hand, we also show that there is a general tradeoff relation between preparational error and fringe visibility, which, for measurements obeying the "non-destruction" condition, reduces to Englert’s inequality.
2:30PM D16.00010 Exact mappings between quantum relativistic and quantum optical models, A. BERMUDEZ et. al, Universidad Complutense de Madrid, E. SOLANO, Ludwig-Maximilians-Universitat — We develop a novel quantum optical perspective into a couple of quantum relativistic systems: i) First we show how the two-dimensional extension of the harmonic oscillator, known as the Dirac oscillator, can be exactly mapped onto a chiral Anti-Jaynes-Cummings model of quantum optics. This equivalence allows us to predict a series of novel relativistic phenomena, such as spin-orbit Zitterbewegung. Furthermore, we also make a realistic experimental proposal, at reach with current technology, for studying the equivalence of both models using a single trapped ion [1], ii) Second, we show that a relativistic version of Schrödinger cat states, here called Dirac cat states, are built in relativistic Landau levels when an external magnetic field couples to a relativistic spin 1/2 charged particle. Under initial suitable conditions, the associated Dirac equation produces unitarily Dirac cat states involving the orbital quanta of the particle in a well defined mesoscopic regime. These states have a purely relativistic origin and cease to exist in the non-relativistic limit [2].

Monday, March 10, 2008 2:30PM - 5:30PM —
Session D16 DBP: Biological Networks Morial Convention Center 208

2:30PM D16.00001 Cooperation of multiple copies of noisy genes, ALEKSANDRA WALCZAK, Princeton University, PETER WOYNES, UCSD — The regulation of gene expression is influenced by the small numbers of protein and gene copies present in the cell. Noise properties arising from single copies of the gene are well known. In this talk we consider the case when a few copies of the same gene are present and actively transcribed in the cell. We use mathematical models which treat both the DNA and protein degrees of freedom stochastically. We study how the switching of one gene influences the switching behaviour of another gene, to which it is coupled by a mutual protein environment. We show that the genes lose properties defined by their individual parameters and take on the characteristics of a group to reach a new steady state. We show that system with multiple gene copies can be used to reduce noise or to modify the cooperativity of the regulatory characteristics of the circuit. These results can be useful for interpreting and designing bioengineering experiments in which there can be multiple copies of a gene.

2:42PM D16.00002 Chaotic Gene Regulatory Networks Can Be Robust Against Mutations and Noise1. VOLKAN SEVIM, PER ARNE RIKVOLD, Florida State University — Robustness to mutations and noise has been shown to evolve through stabilizing selection for optimal phenotypes in model gene regulatory networks. The ability to evolve robust mutants is known to depend on the network architecture. How do the state-space structures of networks with high and low robustness differ? Here we present large-scale computer simulations of a Random Threshold Network model of gene regulatory networks undergoing biological evolution. We show using damage propagation analysis and an extensive statistical analysis of state spaces of these model gene networks that the change in their dynamical properties due to stabilizing selection is very small. Therefore, conventional measures of stability do not provide much information about robustness in model gene regulatory networks. Interestingly, the networks that are most robust to both mutations and noise are highly chaotic. Chaotic networks are able to produce large attractor basins, which can be useful for maintaining a stable gene-expression pattern.

2:54PM D16.00003 A quantitative model of DNA replication in Xenopus embryos: reliable replication despite stochasticity1. SCOTT CHENG-HSIN YANG, JOHN BECHHOEFER, Simon Fraser Univ — DNA synthesis in Xenopus frog embryos initiates stochastically in time at many sites (origins) along the chromosome. Stochastic initiation implies fluctuations in the replication time and may lead to cell death if replication takes longer than the cell cycle time (~25 min.). Surprisingly, although the typical replication time is about 20 min., in vivo experiments show that replication fails to complete only about 1 in 250 times. How is replication timing accurately controlled despite the stochasticity? Biologists have proposed two mechanisms: the first uses a regular spatial distribution of origins, while the second uses randomly located origins but increases their probability of initiation as the cell cycle proceeds. Here, we show that both mechanisms yield similar end-time distributions, implying that regular origin spacing is not needed for control of replication time. Moreover, we show that the experimentally inferred time-dependent initiation rate satisfies the observed low failure probability and nearly optimizes the use of replicative proteins.

3:06PM D16.00004 Exponential sensitivity of noise-driven switching in genetic networks, PANKAJ MEHTA, Princeton University, RANJAN MUKHOPADHYAY, Clark University, NED WINGREEN, Princeton University — Cells are known to utilize biochemical noise to probabilistically switch between distinct gene expression states. We demonstrate that such noise-driven switching is dominated by tails of probability distributions and is therefore exponentially sensitive to changes in physiological parameters such as transcription and translation rates. However, provided mRNA lifetimes are short, switching can still be accurately simulated using protein-only models of gene expression. Exponential sensitivity limits the robustness of noise-driven switching, suggesting cells may use other mechanisms in order to switch reliably.

3:18PM D16.00005 Effects of coarse-graining on fluctuations in gene expression, JUAN PEDRAZA, JOHAN PAULSSON, Department of Systems Biology, Harvard University — Many cellular components are present in such low numbers per cell that random births and deaths of individual molecules can cause significant ‘noise’ in concentrations. But biochemical events do not necessarily occur in steps of individual molecules. Processes are generally randomized when synthesis or degradation occurs in large bursts of many molecules in a short time interval. Conversely, each birth or death of a macromolecule could involve several small steps, creating a memory between individual events. Here we present generalized theory for stochastic gene expression, formulating the variance in protein abundance in terms of the randomness of the individual events, and discuss the effective coarse-graining of the molecular hardware. We show that common molecular mechanisms produce gestation and senescence periods that can reduce noise without changing average abundances, lifetimes, or any concentration-dependent control loops. We also show that single-cell experimental methods that are now commonplace in cell biology do not discriminate between qualitatively different stochastic principles, but that this in turn makes them better suited for identifying which components introduce fluctuations.

3:30PM D16.00006 ABSTRACT WITHDRAWN —
3:42PM D16.00007 Regulatory control and the costs and benefits of biochemical noise. SORIN TANASE-NICOLA, University of Michigan, PIETER REIN TEN WOLDE, Institute for Atomic and Molecular Physics, AMOLF. The Netherlands — Experiments in recent years have vividly demonstrated that gene expression can be highly stochastic. We present a mathematical model that makes it possible to quantify the effect of protein concentration fluctuations on the growth rate of a population of genetically identical cells. The model predicts that the population’s growth rate depends on how the growth rate of a single cell varies with protein concentration, the variance of the protein concentration fluctuations, and the correlation time of these fluctuations. The model shows that when the average concentration of a protein is close to the value that maximizes the growth rate, fluctuations in its concentration always reduce the growth rate. However, when the average protein concentration deviates sufficiently from the optimal level, fluctuations can enhance the growth rate of the population, even when the growth rate of a cell depends linearly on the protein concentration. We also apply our model to perform a cost-benefit analysis of gene regulatory control. Our analysis predicts that the optimal expression level of a gene regulatory protein is determined by the trade-off between the cost of synthesizing the regulatory protein and the benefit of minimizing the fluctuations in the expression of its target gene.

3:54PM D16.00008 Effects of time-delayed negative feedback loops on noise-induced oscillations on the NF-KappaB signaling network. JAEWOOK JOO, JEAN-LOUP PAULON, Sandia National Laboratories — NF-kappaB is a stimulus-responsive pleiotropic regulator of gene control. Our work was motivated by Nelson et al. [Science 306:704 (2004)], which showed noisy quasi-periodic oscillations of NF-kappaB translocation between cytoplasm and nucleus in single cells. Using both stochastic simulations and analytical approaches, we investigated the dynamic patterns of NF-kappaB translocation with a stochastic two-compartamental model, especially taking into account the interplay between intrinsic noise and delayed negative feedback loops of the NF-kappaB signaling system. We will present noise-induced oscillations of the NF-kappaB shuttling and the effects of time-delayed negative feedback loops on them.

4:06PM D16.00009 How is the fitness landscaped upon which life evolves selected? MICHAEL DEEM, Rice University — We investigate the selective forces that promote the emergence of modularity in nature. We demonstrate the spontaneous emergence of modularity in a population of individuals that evolve in a changing environment. We show that the level of modularity correlates with the rapidity and severity of environmental change. The modularity arises as a synergistic response to the noise in the environment, where the presence of horizontal gene transfer facilitates the evolution of hierarchical structures.

4:18PM D16.00010 Early life was a generalist: protein modularity increase as evolution proceeds. JIANKUI HE, JUN SUN, MICHAEL DEEM, Rice University — We study the evolution of modularity in protein-protein interaction network and protein domain-domain interaction networks. By introducing compositional age, we construct the interaction networks at different points in evolutionary time. We use the average-linkage hierarchical clustering method to reorganize the network matrix to identify the modules. With different settings of the compositional age, we compare the observed modularity at different evolutionary times in both E. coli and S. cerevisiae. We conclude that the modularity of protein-protein interaction network and domain-domain interaction network grows in evolution, validating recent theoretical predictions of spontaneous modularity in evolution [1].


4:30PM D16.00011 Genetic recombination models in molecular evolution. ENRIQUE MUNOZ, Department of Physics and Astronomy, Rice University, JEONG-MAN PARK, Rice University and Department of Physics, Catholic University of Korea, MICHAEL DEEM, Department of Physics and Astronomy, Rice University — We introduce generalizations of two classical models of molecular evolution: the parallel or Crow-Kimura model, and the Eigen model. These generalizations include, in addition to point mutations and selection as driving forces for biological evolution, the presence of different forms of horizontal gene transfer and genetic recombination events between individuals in the population. We will present analytical solutions for these models, and compare our results with numerical solutions of the corresponding system of differential equations. We will also present stochastic simulation results for the single peak fitness case.

4:42PM D16.00012 A minimal stochastic model of cell death signaling. SUBHADIP RAYCHAUDHURI — Cell death (apoptosis) is mediated by a complex intracellular signaling network that involves a large number of components. We propose a minimal model of signaling network that can sense the strength of any extracellular stimuli such as the concentration of ligands and adapt to a fluctuating environment. Based on stochastic simulations we show that a three step slow, fast, slow pathway is enough to generate large cell to cell fluctuations under the conditions of weak stimulus. Such cell to cell stochastic fluctuations persist even in the presence of large number of molecules and cannot be captured by deterministic differential equations. The model is based on stochastic simulations. We develop a probability distribution based approach that can characterize the stochastic fluctuations in such inherently stochastic signaling network. Interestingly, our results match with those obtained from kinetic Monte Carlo simulation of the full scale apoptotic network. Hence, our minimal signaling network can serve as a cell type independent general model of apoptosis signaling. We also discuss implications of our probability distribution based approach for diseases such as cancer that can result from disrupted apoptotic balance.

4:54PM D16.00013 Temperature compensation model for the circadian clock of Neurospora crassa.1 XIAOJIA TANG, HEINZ-BERND SCHÜTTLER, Department of Physics and Astronomy, University of Georgia, JONATHAN ARNOLD, Department of Genetics, University of Georgia — In the lowly bread mould, Neurospora crassa, biomolecular reactions involving the white-collar-1 (wc-1), white-collar-2 (wc2), and frequency (frq) genes and their products constitute building blocks of the biological clock that would respond to temperature as well as light. The frequency of the biological clock remains stable in response to variation in ambient temperature, which is called a compensation phenomenon. Recent experimental results show evidences that the temperature compensation could be explained by the temperature sensitive translational control of production of two isoforms of the main oscillator protein FRQ: a long form FRQ and a short form FRQ, which are more abundantly produced at higher temperature; and a short form FRQ, which is more abundantly produced at lower temperature. With our recently developed method of genetic network identification, we are now simulating the network’s temperature response based on published experimental data. These will serve as the starting point for a simulation-prediction-experiment-simulation workflow cycle. In this cycle, the maximally informative next experiment (MINE) technology will be employed to select the best experimental control parameters specifying the temperature response to be used in the next step of the workflow cycle.

1) NSF BES-0425762.

5:06PM D16.00014 Understanding the Role of Housekeeping and Stress-Related Genes in Transcription-Regulatory Networks. ALLISON HEATH, LYDIA KAVRAKI, Rice University, GÁBOR BALÁZSI, University of Texas M.D. Anderson Cancer Center — Despite the increasing number of completely sequenced genomes, much remains to be learned about how living cells process environmental information and respond to changes in their surroundings. Accumulating evidence indicates that eukaryotic and prokaryotic genes can be classified in two distinct categories that we will call class I and class II. Class I genes are housekeeping genes, often characterized by stable, noise resistant expression levels. In contrast, class II genes are stress-related genes and often have noisy, unstable expression levels. In this work we analyze the large scale transcription-regulatory networks (TNR) of E. coli and S. cerevisiae and preliminary data on H. sapien. We find that stable, housekeeping genes (class I) are preferentially utilized as transcriptional inputs while stress related, unstable genes (class II) are utilized as transcriptional integrators. This might be the result of convergent evolution that placed the appropriate genes in the appropriate locations within transcriptional networks according to some fundamental principles that govern cellular information processing.
5:18PM D16.00015 The re-design of a theophylline riboswitch for DNT sensing1, YAROSLAV CHUSHAK, Biotechnology HPC Software Applications Institute, USAMRMC, NANCY KELLEY-LOUGHNAINE, SVETLANA HARBALGA, MORLEY STONE, Air Force Research Laboratory, Wright-Patterson AFB — Riboswitches are noncoding elements of mRNA that recognize and bind to small molecules and regulate the translation process of downstream genes. As an initial study, we used a theophylline riboswitch that regulates the expression of the Tobacco etch virus (TEV) protease placed downstream of the switch as a controlling element. Upon expression of TEV protease, an optical reporter is cleaved producing change in fluorescence resonance energy transfer (FRET) between BFP and eGFP. We altered the sensing domain of the original construct to create a synthetic riboswitch that responds to the presence of 2,4-dinitrotoluene (DNT) molecules. Computational analysis using AutoDock4 and AMBER9 software packages showed that U24A mutant has a significantly higher binding affinity for DNT molecule compared to the original theophylline. Cells expressing the re-designed riboswitch showed a marked optical difference in emission in the presence of DNT molecules, leading to the potential of using this construct in biosensitonal applications of highly nitrated compounds.

1This work was supported by the Air Force Office of Scientific Research (AFOSR) and by the DOD HPC Modernization Program (HPCMP).

Monday, March 10, 2008 2:30PM - 5:30PM — Session D17 DBP: Focus Session: Time-Resolved Structural Investigations on Protein Folding and Function Morial Convention Center 209

2:30PM D17.00001 Folding dynamics of a family of beta-sheet proteins1, DENIS ROUSSEAU, Albert Einstein College of Medicine — Fatty acid binding proteins (FABP) consist of ten anti-parallel beta strands and two small alpha helices. The beta strands are arranged into two nearly orthogonal five-strand beta sheets that surround the interior cavity, which binds unsaturated long-chain fatty acids. In the brain isoform (BFABP), these are very important for the development of the central nervous system and neuron differentiation. Furthermore, BFABP is implicated in the pathogenesis of a variety of human diseases including cancer and neuronal degenerative disorders. In this work, site-directed spin labeling combined with EPR techniques have been used to study the folding mechanism of BFABP. In the first series of studies, we labeled the two Cys residues at position 5 and 80 in the wild type protein with an EPR spin marker; in addition, two singly labeled mutants at positions 5 and 80 in the C80A and C5A mutants, respectively, were also produced and used as controls. The changes in the distances between the two residues were examined by a pulsed EPR method. DEER (Double Electron Electron Resonance), as a function of guanidinium hydrochloride concentration. The results were compared with those from CW EPR, circular dichroism and fluorescence measurements, which provide the information regarding sidechain mobility, secondary structure and tertiary structure, respectively. The results will be discussed in the context of the folding mechanism of the family of fatty acid binding proteins.

1This work was supported by the National Institutes of Health. The coauthors are Makiko Uchida, Gary Gerfen and Syun-Ru Yeh.

3:06PM D17.00002 Ultrafast studies of flavins and flavoproteins, DONGPING ZHONG, Dept. of Physics, The Ohio State University — Flavin molecule plays an essential role as a cofactor in flavoproteins with its rich redox states. We have systematically studied the excited-state dynamics of three different redox states (oxidized, semiquinone, and fully reduced) in bulk solvent and in some important proteins. A series of new results were obtained and a correlation of structure-redox-dynamics-function in proteins was observed. We use two important proteins, photolyase and flavodoxin, to show these significant findings.

3:42PM D17.00003 Coupled folding and binding kinetics in the intrinsically disordered peptide IA31, RANJANI NARAYANAN, Department of Physics, University of Florida, OMJOY GANESH, ARTHUR EDISON, Department of Biochemistry and Molecular Biology, University of Florida, STEPHEN HAGEN, Department of Physics, University of Florida — IA3 is an intrinsically disordered 68 residue peptide and is an endogenous inhibitor of yeast peptidase A (YPaA). X-ray crystallography of the IA3-YPaA complex [Li et al, Nat. Struct. Biol. (7), 113-117 (2000)] indicates that the N-terminus of IA3 adopts an alpha-helical fold when it is bound to the YPaA active site. We have used equilibrium circular dichroism and multi-wavelength, nanosecond time-resolved laser temperature-jump spectroscopy to study the coupled folding and binding interaction of IA3 with YPaA. Our initial measurements of the rate of helix formation in free IA3 indicate mono-exponential folding kinetics that extrapolate to kF ~ 107/s at room temperature in aqueous solutions. By comparing this rate to the kinetics we observe for IA3 interacting with YPaA, we can assess possible mechanisms for the coupled folding and binding of IA3.

1Supported by NSF MCB # 0347124.

3:54PM D17.00004 Impact of Salt and Water on Protein Structural Dynamics, ANU THUBAGERE, LORAND KELEMEN, BEINING NIE, SANDIP KALEDHONKAR, AIHUA XIE, Oklahoma State University — Water is known as the lubricant of life. Without water, most proteins would lose their biological functions. Extensive studies have been carried out on how high concentration salts (dissolved in water) alter the stability and solubility of proteins. Such effects are thought to be mediated via salt-water interactions and water-protein interactions. This classic research field is known as the Hofmeister Series. We report the effects of Hofmeister Salts on the structural dynamics of proteins. Photoactive yellow protein (PYP), a bacterial blue light photoreceptor protein, is employed as a model system in this study. Time-resolved FTIR spectroscopic techniques allow us to probe the structural changes in proteins. Our data reveal that high concentration salt solutions alter the proton transfer pathway and suppress conformational changes in PYP upon photo-excitation. This study opens up a new dimension in the field of Hofmeister series. Further theoretical and experimental studies are needed in order to understand the dynamic properties of salt-water interactions and water-protein interactions.

4:06PM D17.00005 Direct protein photoinduced conformational changes using porphyrins, LORENZO BRANCALEON, IVAN SILVA, NICOLAS FERNANDEZ, ERIC JOHNSON, SAMUEL SANSONE, University of Texas at San Antonio — Most proteins functions depend on their interaction with other ligands. This interactions depend on uniquely structured binding sites formed by the folding of the proteins. Ligands can often prompt intended as well as “accidental” protein structural changes. One can foresee that the ability to prompt and control post-translational protein folding could be a powerful tool to investigate protein folding mechanisms but also to inhibit certain proteins or induce new properties to proteins. One possible way to produce such structural disruption is the combination of light and photoactive ligands. This option has been investigated in recent years by exploiting photosomerization and other properties of non-physiological dyes. We used an alternative approach which uses porphyrins as the “triggers” of structural changes. The advantage of porphyrins is that they can be found naturally in living cells. The photophysical properties of porphyrins can induce local as well as long range effects on the structure of the bound protein. Porphyrins are known to produce structural changes in porphyrin-specific globular proteins, however the novelty of our results is that we demonstrated that these dyes can also produce structural changes in non-porphyrin-specific globular proteins. We will present an overview of our research to-date in this field and its potential applications.
4:18PM D17.00006 Computer simulations of the folding mechanism of the GCN4 Leucine zipper, YANXIN LIU, PREM CHAPAGAIN, JOSE PARRA, BERNARD GERSTMAN, Department of Physics, Florida International University, University Park, Miami, FL 33199 — A modified three-dimensional lattice model incorporating a Monte Carlo Metropolis Algorithm is used to investigate the dimerization of the GCN4 Leucine zipper. The model is validated with heat capacity calculations that are seen to match well with experiment measurements. The free energy landscape is investigated as a function of temperature. Evidence of multiple meta-stable states is found during the simulation. The possible folding and dimerization mechanism of the Leucine zipper will be discussed.

1Department of Physics, University of Florida, Gainesville, FL 32611

4:30PM D17.00007 Describing protein folding through the evolution of spatial density, XIANG-HONG QI, JOHN J. PORTMAN, Kent State University — The capillary-like structure of folding nuclei is directly characterized for a wide range of two state folding proteins within a variational model that includes “neutral” cooperativity. We find that on average the volume of the folded core depends on the number of monomers as \( V_f \sim N^{0.3} \). The precise relation agrees with the packing of rigid objects that are typically twice the size of a monomer in the native state. Focusing on the growth of the folded core and the interface region, we identify three different growth modes: core and interface consolidation, core dominated consolidation, and balanced growth. We also show in detail how the density of the core and interface of critical nuclei determine the common qualitative characterization as either diffuse or polarized. Such analysis will aid interpretation of \( \phi \)-value distributions in terms of the spatial density or compactness of the critical nucleus which is much more difficult to probe experimentally than the degree of similarity to the native state.

4:42PM D17.00008 The trigger sequence in the protein folding and dimerization of the Leucine zipper coiled-coil motif, PREM CHAPAGAIN, YANXIN LIU, BERNARD GERSTMAN, Department of Physics, Florida International University, University Park, Miami, FL 33199 — The existence of a trigger sequence in the protein folding and dimerization of the Leucine zipper coiled-coil structure is attracting increased interest. Also of interest is the presence of multiple meta-stable states in the folding and unfolding process. Using a computer lattice model, we investigate the effect of the trigger sequence by changing the strength of the propensity of the amino acids in the trigger sequence to form alpha-helix secondary structure. The results show that the trigger sequence is necessary for folding and dimerization. The trigger sequence also creates a folding and dimerization process that includes multiple meta-stable states.

4:54PM D17.00009 Correlation functions of flexible macromolecules, DONALD JACOBS, DENNIS LIVESAY, OLEG VOROV, UNC at Charlotte — We present an ab initio calculation of conformational entropy, radii of gyration, X-ray and neutron scattering form-factors, correlation functions, and other observables describing proteins, polypeptides, nucleic acids, related macromolecules and artificial polymers [1]. The analytic form of the method minimizes computational costs and reveals relations between observables. We apply these methods to study thermodynamics of protein unfolding. The presented results agree with the results from experiment and simulation [2].


Supported by NIH grant NIGMS R01 GM073082-01A1

5:06PM D17.00010 ABSTRACT WITHDRAWN

5:18PM D17.00011 Photocycle of a single photoactive yellow protein molecule studied by surface-enhanced Raman scattering, KAAN KALKAN, KUSHAGRA SINGHAL, WOUTER HOFF, AIHUA XIE, Oklahoma State University — We have demonstrated the detection of single molecules of photoactive yellow protein (PYP), by employing our novel surface-enhanced Raman scattering (SERS) active substrates. The Raman spectra reveal both “receptor” (G) and “signaling” (B) states of PYP at the single molecule level (at 514 nm excitation). The single molecule spectra are observed in terms of sudden appearance of discernable Raman peaks, each indicative of a PYP molecule finding a hot spot. The SERS spectra also exhibit various peaks, which are not normally Raman-active. Although the PYP has a long-lived signaling state (i.e., \( \sim 0.3 \) s), the Raman peaks identifying this state are found to be dramatically narrow at the single molecule level for signal integration times of 0.25-0.5 s. In several instances, we observed subsequent change of the spectrum from B to G state. Although, the PYP is not chemisorbed on the metal nanoparticles, its short-term psysorption is anticipated to allow for the capture of its photocycle at the single molecule level. In addition to narrower and better resolved peaks, the single molecule spectra also show variation in relative peak intensities. In particular, the C-C stretching and C-H bending modes of the aromatic ring of the chromophore inversely correlate at the single molecule level, while their intensities are comparable in the ensemble-average spectrum.

Monday, March 10, 2008 2:30PM - 5:30PM
Session D18 DPOLY: Polymers at Surfaces Morial Convention Center 210

2:30PM D18.00001 Surface Segregation in Blends of Chains with Two Architectures, MARK FOSTER, SEWOO YANG, NAM-HEUI LEE, The University of Akron, DAVID WU, Colorado School of Mines — Blends of chains of two architectures, e.g. linear chains with pom-pom branched polymers, present opportunities for tailoring bulk rheology and surface character of the blends. Pom-pom chains contain a central linear portion between two junction points from which multiple arms extend. We have studied the effect of varying the relative length of the central linear portion between two junction points from which multiple arms extend. The strength of segregation to the surface and substrate interface of a blend film is seen with neutron reflectivity and surface enhanced Raman spectroscopy to correlate at the single molecule level, while their intensities are comparable in the ensemble-average spectrum.

1Supported by NSF CBET-0730692 and Ohio Board of Regents Challenge Grant

2:42PM D18.00002 Single chain mobility at an interface of a liquid polymer, JINGFA YANG, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — Interfacial diffusion of single chains of polystyrene-b-polyisoprene (PS-b-PI) at the interface between polystyrene and its non-solvent, DMF, was studied by fluorescence correlation spectroscopy. The diffusion coefficient of PS-b-PI probe was found to be two orders of magnitude high than that in the bulk PI, indicating a lower interfacial viscosity. The experimental data also exhibit a very weak dependence of the interfacial diffusion coefficient on the molecular weight of the liquid polymer. The possible mechanism was discussed.

1Project supported by The National Natural Science Foundation of China (NSFC) and the Ministry of Science and Technology of China (MOST)
2:54PM D18.00003 Molecular origin of oil resistance of polyacrylonitrile: CN interactions at the surface . VERONIQUE LACHAT, ALI DHINO.IWAL. The University of Akron, DENNIS PEIFFER, MOHSEN YEGANEH, ExxonMobil Corporate Strategic Research Laboratories — Nitrile rubber (NR) is a random copolymer of acrylonitrile and butadiene and is one of the best oil resistance polymers. The superior oil resistance property of nitrile rubber is thought to be directly related to the amount of acrylonitrile used in NR. Here, we report for the first time measurements on materials that fit this description, C_60 reaction conditions was found to influence the observed coverage kinetics, so film swelling was monitored with environmental AFM. The attachment to these surfaces follow different kinetics than those observed for the polymeric substrates. The swelling of the polymeric substrates under the increasing AA and nanoparticle concentration, and time. SAMs containing an acrylic acid moiety were used as a non-swelling control surface, and particle (SAMs) of (3-aminopropyl)triethoxysilane were covalently attached to the PS-ran-PAA films with an EDC/NHS coupling reaction. To measure the kinetics of efforts have focused on the development of nanoparticle arrays with controlled spacing. In this study, poly(styrene-ran-acrylic acid) films were prepared by spin-

3:06PM D18.00004 Effect of Hydrogen Bonding on Colloidal Nanocrystal Growth: The Case for PbS . LIXIN ZHANG, National Renewable Energy Laboratory, Golden, CO 80401, SHENGBAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180 — The adsorption of methylamine (CH_3NH_2) on rocksalt PbS(111)-S surface is studied by first-principles total energy calculation. It was found that nitrogen lone pairs on the CH_3NH_2 can form dative bonds with surface sulfur atoms. Such an interaction is unique in two ways: first it is non-local. Charge transfer takes place from CH_3NH2 not only to the closest S but also to surface S further away. Second, the interaction is strongly affected by hydrogen bonds formed between CH_3NH2 and solution molecules such as H_2O. Only by the latter effect can the PbS nanocrystals assume the (111) facets in a colloidal growth in agreement with experiment. In the past, studies of nanostructures have taken the assumption that, in the absence of a solution, the relative stability among the various facets will not change, at least not dramatically. Our study shows that such an assumption is not necessarily true. The significance of the study therefore goes beyond just the PbS or PbTe systems. Its basic principles should apply to all colloidal growth of solid-state nanostructures with broad implications.

3:18PM D18.00005 Conformational behavior of polymers adsorbed on nanotubes . SIMCHA SREBNIK, INNA GUREVITZ, Technion - Israel Institute of Technology — We study the interaction of a dilute solution of semiflexible polymers with a weakly attractive infinitely long nanotube using Monte Carlo simulation. Apart for bending stiffness of the polymer chains, the only interactions considered in our model are weakly attractive short-ranged Lennard-Jones interactions between the monomers and with the surface. These nonspecific interactions are found to result in stable helical and multi-helical adsorbed conformations for semiflexible chains. Adsorption of these chains is found to occur in a sequential manner through tight wrapping of the polymer around the nanotube. Adsorption occurs quickly and is characterized by a sharp peak in the heat capacity. A second transition follows whereby opening and reorganization of the adsorbed chains into nearly perfect helices and multiple helices. Extension of the model to block and triblock copolymers reveals rich conformational behavior. These results are discussed on physical grounds and implications towards polymer-carbon nanotubes composites are offered.

3:30PM D18.00006 Origin of glass transition temperature behavior in polymer nanocomposites . JAMIE KROPKA, VENKAT GANESAN, The University of Texas at Austin, PETER GREEN, The University of Michigan — Local composition variations inherent in multi-component materials, even when the material constituents are miscible, generally lead to heterogeneous behavior in the properties of mixtures relative to their single component counterparts. In contrast, experiments have suggested that some polymer nanocomposite materials exhibit changes in their bulk T_g without displaying excess heterogeneity in their dynamics, as measured mechanically, relative to the neat polymer. Incoherent neutron scattering measurements for blends of PMMA and PPO, and this model for PMMA mixtures, suggest that modifications of the polymer melt dynamics are limited to the vicinity of the particles. A model by which the localized modifications of polymer dynamics can account for the apparent homogeneous change in T_g is proposed to explain the experimental findings. Computations based on percolation theory support the model.

3:42PM D18.00007 Directed Self-Assembly of Gradient Concentric Carbon Nanotube Rings . SUCK WON HONG, WONJE JEONG, Iowa State University, HYUNHYUB KO, VLADIMIR TSUKRUK, Georgia Institute of Technology, MICHAEL KESSLER, ZHIQUN LIN, Iowa State University — Hundreds of gradient concentric rings of linear conjugated polymer, (poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene], i.e., MEH-PPV) with remarkable regularity over large areas were produced by controlled, repetitive “stick-slip” motions of the contact line in a confined geometry consisting of a sphere on a flat substrate (i.e., sphere-on-flat geometry). Subsequently, MEH-PPV rings exploited as template to direct the formation of gradient concentric rings of multiwalled carbon nanotubes (MWNTs) with controlled density. This method is simple, cost effective, and robust, combining two consecutive self-assembly processes, namely, evaporation-induced self-assembly of polymers in a sphere-on-flat geometry, followed by subsequent directed self-assembly of MWNTs on the polymer-templated surfaces.

3:54PM D18.00008 Use of Fluorescence Correlation Spectroscopy for Studying Polyelectrolyte-Nanoparticle Interaction in Aqueous Solution . NADIA EDWIN, DENIS PRISTINSKI, CHENGQING WANG, VIVEK PRABHU, NIST — Formation of polyelectrolyte complexes is very facile via layer-by-layer sequential adsorption of oppositely charged species method. This method has been used to fabricate versatile materials with tailored properties. However, the fundamental assembly mechanisms of these advanced engineering materials and the adsorption kinetics of these systems is not completely understood. We use fluorescence correlation spectroscopy (FCS), which analyzes fluctuations in the fluorescence emission of molecular ensembles and provides the concentration, mobility, and dynamics of fluorescently labeled molecules, to study the interaction of polyelectrolyte-nanoparticle assembled structures to establish what’s driving the adsorption of these systems, the dependence of molecular weight and the effects of variations in the solution environment with pH and ionic strength. Layer-by-layer assembly was performed on fluorescent dye-labeled spherical nanoparticles and amine and carboxyl functionalized polyelectrolytes in aqueous solution. Changes in the dynamics of the polyelectrolyte-nanoparticle system in response to various salt and pH conditions will be presented.

4:06PM D18.00009 Directed Nanoparticle Assembly onto Random Copolymer Templates: Kinetics and Surface Considerations . MARLA MCONNELL, SHU YANG, RUSSELL COMPOSTO, University of Pennsylvania — Recent efforts have focused on the development of nanoparticle arrays with controlled spacing. In this study, poly(styrene-ran-acrylic acid) films were prepared by spin-casting poly(styrene-ran-t-butyl acrylate), followed by thermal deprotection. Silica nanoparticles (10-15 nm in diameter) coated with self-assembled monolayers (SAMs) of (3-aminopropyl)triethoxysilane were covalently attached to the PS-ran-PAAc films with an EDC/NHS coupling reaction. To measure the kinetics of nanoparticle attachment, films of either 25 or 50 weight percent acrylic acid were reacted with nanoparticle suspensions from 0.005 to 0.1 weight percent for varying lengths of time. SEM imaging of the nanoparticle surfaces showed that the particles were well dispersed, and that particle coverage increased with increasing AA and nanoparticle concentration, and time. SAMs containing an acrylic acid moiety were used as a non-swelling control surface, and particle attachment to these surfaces follow different kinetics than those observed for the polynimeric substrates. The swelling of the polynimeric substrates under the reaction conditions was found to influence the observed coverage kinetics, so film swelling was monitored with environmental AFM.
4:18PM D18.00010 Studies of the Dynamics of Alkane Nanoparticles1, S.-K. WANG, M. BAI, H. TAUB, M. RHEINSTADTER, U. Mo.-Columbia, J. R. D. COLEY, V. GARCIA SAKAI, G. GASPAROVIC, NIST, U. C. VOLKMAN, P. U. Catolica Chile, P. Y. HANSEN, Tech. U. of Denmark — Our AFM and synchrotron x-ray scattering measurements on dotriacontane (C32H66 or C32) deposited on SiO2-coated Si(100) substrates reveal mesa-shaped nanoparticles that have an orthorhombic structure in which the C32 molecules are aligned perpendicular to the SiO2 surface. To investigate their dynamical properties, we have used both the backscattering and disk chopper spectrometers at NIST covering a wide range of time scales (1 ps – 4 ns). Elastic scans obtained on both spectrometers show step-like changes in intensity as a function of temperature indicating the existence of phase transitions below the bulk C32 melting point. One of these steps occurs at the crystalline-to-rotator phase transition of bulk C32, but there is a second step at still lower temperature of unknown origin. The similarity of the elastic scans on the two spectrometers suggests that the crystalline-to-rotator phase transition involves diffuse motion spanning a wide range of time scales. #M. Bai et al., Europhys. Lett. 79, 26003 (2007).

1Supported by Grant Nos. U.S. NSF DMR-0411748 and DMR-0705974, by the U.S. DOE through Grant No. DE-FG02-01ER45912, and FONDECYT 1060628 and 7070248.

4:30PM D18.00011 Hierarchically Ordered Plasmonic Mask for Photo-lithography . WOO SOO KIM, EDWYN L. THOMAS, MIT — A new high density nanolithography method for the fabrication of a hierarchically ordered plasmonic mask employs silver (Ag) nano-particles (NPs) attached to the surface of an amine- functionalized two-dimensional (2D) pattern fabricated by laser interference lithography (IL). The bi-functional sol-gel hybrid material (BFHM) is a negative-tone resist and can be directly patterned by IL. Since the BFHM has both an amine-function and a methacryl function on each polymer chain, photopolymerization provides network formation and a set of binding sites for the Ag NPs. The Ag NPs were then attached onto the BFHM pillars by immersing the patterned sample in a solution. Hierarchically ordered arrays of Ag NPs could be made by a block copolymer comprised of 40nm diameter spherical P2VP domains having a spacing of 88nm, forming a hexagonal pattern covering the hexagonally arrayed BFHM pillars. Lithography experiments using 430 nm light wavelength demonstrate transfer of both a 350 nm periodic pattern and a 88nm patten to a positive-tone photoresist via plasmonic field enhancement arising from the collective and individual excitation of the closely spaced interacting Ag NPs on the hierarchically patterned BFHM.

4:42PM D18.00012 Dynamics of an Adsorbed Polymer Chain . JOSHUA KALB, SANAT KUMAR, Columbia University — Because of the current precision in fluorescent labeling, it is possible to label single polymers such as DNA or PEG and track their dynamical and equilibrium properties in the bulk as well as near attractive surfaces [Maier et. al., Macro 2000] [Sukhishvili et. al., Macro 2002]. Recent evidence from these experiments and related simulations has shown that the dynamics of a single polymer near an attractive surface appear diffusive, however further evidence coming from the ‘diffusion coefficient’ implies a different process other than diffusion is at work such as reptation, ‘hovercrafting’, or ‘hopping’ [Sukhishvili et. al., Macro 2002]. In general, these possible dynamical behaviors are determined by the length of the polymer itself as well as the microscopic details of the attractive surface which include the density, strength, and distribution of attractive surface sites [Desai et. al., PRL 2007] [Qian et. al., PRL 2007]. In this presentation, we investigate the effects of microscopic surface effects on single polymer dynamics through Monte-Carlo and molecular dynamics simulations.

4:54PM D18.00013 Chasing drops: Following escaper and pursuer drop couple systems . AISHA LEH, RAFAEL TADMOR, PREETI YADAV, PRASHANT BHADUR, KUMUD CHAUDRASIA, LAN DANG, Lamar University — We study the Marangoni flow induced by two chemically different drops resting on a solid surface in air. We show that in all the systems studied, the Marangoni flow is induced at the solid-liquid interface as opposed to the air-liquid interface. This is true even for the case of water drop and alcohol drop on a glass surface (corresponding to the classical “tears of wine” case). Thus we explain the drop motion as a result of a surface tension gradient which takes place primarily at the air-surface region (and less at the drop-substrate or drop-air interfaces). The discontinuous motion of the drops, characterized by stops and jumps as in a “stick slip” mechanism is explained by an increase in the Laplace pressure that creates a higher anchoring pinning effect at the front edge of the moving drop. We discuss this in connection to the “tears of wine” case.

5:06PM D18.00014 The Measurement of Surface Rheological and Surface Adhesive Properties using Nanosphere Embedment . STEPHEN HUTCHESON, GREGORY MCKENNA, Department of Chemical Engineering - Texas Tech University — In previous work, we determined the actual rheological behavior at the surface of a polystyrene film with nanometer scale resolution by applying a viscoelastic contact mechanics model to experimental data in the literature. The goal of our current research is to build upon this analysis and use nanosphere embedment experiments to probe the nanorheological behavior of polymer surfaces near the glass transition, in the melt state and in the solid rubbery state. An atomic force microscope (AFM) is used to probe the embedment depth as nanoparticles are pulled into the surface by the thermodynamic work of adhesion. The results show that, with properly designed experiments, both the surface adhesion properties and the surface rheological properties can be extracted from nanosphere embedment rates. We include work on a phase separated copolymer and a commercially available polydimethylsiloxane (PDMS) rubber.

5:18PM D18.00015 Slip behavior of the confined polymer melt near periodically roughened surfaces: comparison between molecular dynamics and continuum simulations . ANOOSHEH NIAVARANI, NIKOLAI PRIEZJEV, Michigan State University — Molecular dynamics (MD) simulations are used to investigate the behavior of the slip length in the Couette flow of a polymer melt. For atomically smooth surfaces and weak wall-fluid interactions, the shear rate dependence of the slip length is a non-monotonic function, with a distinct local minimum. For corrugation wavelengths larger than the radius of gyration of polymers, the decay of the slip length with corrugation amplitude obtained from MD simulations agrees well with the continuum predictions for the following cases: (1) Stokes solution with constant local slip length, (2) Stokes solution with local shear-rate-dependent slip length, and (3) Navier- Stokes solution with local rate-dependent slip length. If the corrugation wavelength is less than or on the order of the radius of gyration, the continuum predictions (the Stokes solution) overestimate the values of the slip length extracted from MD simulations. The analysis of the conformational properties of the polymer melt indicates that polymer chains tend to stretch in the direction of shear at the peaks of the sinusoidal wave and align themselves along the bottom of the grooves.

Monday, March 10, 2008 2:30PM - 5:30PM
Session D19 DMP: Focus Session: Dopants and Defects in Semiconductors 1 Morial Convention Center 211
2:30PM D19.00001 Stability and Dynamics of Frenkel Pairs in Silicon

MATTIEW J. BECK, Physics and Astronomy, Vanderbilt University — Extensive EPR experiments on electron irradiated p-Si observe only signals identified as arising from isolated vacancies and interstitial impurities. Subsequent experiments and calculations demonstrated that isolated interstitials in p-Si diffuse athermally according to a charge-carrier-mediated mechanism. The overall conclusion has been that Si FPs either rapidly recombine or dissociate, even at cryogenic temperatures. More recent X-ray scattering experiments, however, suggest that Si FPs persist at temperatures up to 150 K. We report first-principles calculations of Si FP properties and resolve the apparent conflict between experiments. We find that the vacancy and interstitial components of a proximal FP interact electronically, suppressing the previously identified athermal interstitial diffusion. Such proximal FPs are bound only by the presence of barriers to either recombination or dissociation.

Further, metastable FPs may lower their energy by transferring electrons from the interstitial to the vacancy component. We show that EPR studies of FPs are likely unable to distinguish between FPs and isolated vacancies. In addition, calculated diffusion barriers for FP components indicate that FPs should anneal at temperatures similar to those for isolated vacancies: \( \sim 150 \) K.

1 Collaborators: L. Tsetseris and S. T. Pantelides; this work was supported in part by the AFOSR through a MURI grant.

3:06PM D19.00002 Defect Formation Energies without the Band-Gap Problem: Combining DFT and GW for the Silicon Self-Interstitial

P. RINKE, A. JANOTTI, C.G. VAN DEWALLE, M. SCHIEFFLER, University of California at Santa Barbara — For the self-interstitial in silicon, a defect of high technological relevance, density functional theory (DFT) in the widely applied local-density approximation (LDA) underestimate the formation energies of different configurations in the neutral charge state by \( \sim 1.5 \) eV compared to diffusion Monte Carlo calculations [1,2]. We attribute this to artificial self-interaction and the absence of the derivative discontinuity in the LDA-exchange-correlation potential that give rise to the band-gap problem. We present a new formalism that combines LDA with quasiparticle energy calculations in the \( G_0W_0 \) approximation to overcome these deficiencies. The formation of the neutral defect is expressed as successive charging of its 2\(^+\) charge state, for which the defect level is unoccupied, permitting a decomposition into a lattice (LDA) and an electron addition part (\( G_0W_0 \)) [3]. The \( G_0W_0 \) corrections increase the LDA formation energy by \( \sim 1.1 \) eV. Moreover, the \( G_0W_0 \)-corrected charge transition levels agree well with recent measurements [4]. [1] Batista et al. PRB 74, 121102(R) (2006), [2] Leung et al. PRL 83, 2351 (1999), [3] Hedström et al. PRL 97, 226401 (2006), [4] Bracht et al. PRB 75, 035211 (2007)


AMITA WADEHRA, JOHN W. WILKINS, Ohio State University, RICHARD G. HENNIG, Cornell University — The self-interstitials in silicon created by ion-beam processing determine migration rate of impurities, time evolution of dislocations and dopant-enhanced diffusion. The large mobility of interstitials makes their experimental observation difficult. Electron-assisted transport mechanism suggests that charged states with different migration barriers and minimum energy positions are responsible for this rapid migration. Therefore, it becomes necessary to identify the stable ground state charges for each geometry and electron chemical potential. Recent studies of energetics and migration of these defects have largely concentrated on neutral defects and a few on charged single interstitials. We present a density functional study of electronic structure and energetics of charged single-, di- and tri-interstitials in silicon. An analysis of stability of five different charged states in various geometries is provided through formation energies. The diffusion pathways of these charged interstitials are also discussed.

3:30PM D19.00004 Large scale ab initio calculations for shallow acceptor levels in bulk Si

LIN-WANG WANG, Lawrence Berkeley National Laboratory — Accurate calculation of shallow donor levels in conventional semiconductors is a long standing challenge due to the large supercell needed for such calculation. We have used the charge patching method and local density approximation (LDA) to study the acceptor levels in bulk Si, including B, Al, Ga, In and Ti acceptors. The atomic positions are relaxed under LDA using 512 atom cells, and 64,000 atom supercells are used to calculate the acceptor energy levels to achieve the converged results. The calculated impurity binding energies reproduce the experimental trend from B to Ti. However, there is still a significant difference between the calculated binding energies and the experimental results, especially for Ti. This raises the question of whether the LDA can be used to calculate the shallow impurity level accurately.

1 This work is supported by U.S. Department of Energy, BES, under contract No. DE-AC02-05CH11231 and it used the resource of the National Energy Research Scientific Computing Center.

3:42PM D19.00005 Relative stability of extended interstitial defects in silicon: large-scale classical MD and first-principles DFT

HYOUNGKI PARK, JOHN WILKINS, The Ohio State University — Extensive simulations for doped Si reveal the relative thermal and temporal stability of extended interstitial defects: 311 and 111 rod-like defects, and Frank dislocation loops. Classical molecular dynamics simulations provide the atomic configurations of those defects, and show that the energetically favored structures change from 311 rod-like defects to Frank loops as the number of interstitials increases, which is consistent with the experimentally-observed transition from rod-like defects to Frank loops after long, high-temperature annealing processes [1,2]. This relative stability is validated with massively parallelized density-functional calculations of 1500-atoms 2D supercells. Relaxation of experimentally-observed-size defect cluster demonstrates the energetic hierarchy is dependent on the number of interstitials in the defect clusters. [1] L. S. Robertson et al., J. Appl. Phys. 87, 2910 (2000). [2] G. Z. Pan et al., J. Non-Crystalline Solids 352, 2506 (2006).

3:54PM D19.00006 Ortho-para transition of interstitial H\(_2\) in Si

MICHAEL STAVOLA, CHAO PENG, MEGAN LOCKWOOD, Lehigh University — Interstitial H\(_2\) in Si is a nearly-free rotator and has ortho and para species with the nuclear spins of the two protons aligned either parallel or antiparallel [1]. If one waits a sufficiently long time at low temperature, H\(_2\) will relax to its lower energy para state. The ortho-para (o-p) transition for H\(_2\) in Si has been observed in recent Raman studies [2]. We have performed IR absorption experiments to investigate issues that have proved difficult to study by Raman. When a Si sample containing H\(_2\) is stored for a month or more at 77K, the 3618.4 cm\(^{-1}\) IR line assigned to o-H\(_2\) [1] is reduced in intensity because, when the o-p transition occurs, p-H\(_2\) is not seen by IR. When this sample was annealed at room temperature, the ortho population characteristic of room temperature was recovered with a time constant of \( \sim 6\) hrs. Our IR studies of the kinetics of the o-p transition complement recent Raman results and suggest that the cause of the o-p transition is not yet understood.


1 Supported by NSF grant no. DMR 0403641.
4:06PM D19.00007 Carbon Impurity Effects on Structural and Magnetic Properties of Manganesne Doped Silicon, JOSHUA LAROSE, ROGER PINK, TARA P. DAS, MENG-BING HUANG, SUNY-Albany, JIAN-QING WANG, SUNY-Binghamton — The recent finding of room temperature ferromagnetism in Mn-doped Si may open up a promising route toward Si-based spintronic. In this work, we investigate effects of co-doped carbon on the structural and magnetic properties of Si:Mn, in a hope to identify possible microstructures responsible for ferromagnetism. Carbon atoms of 0.25 at. % are uniformly doped within the 200-nm surface layer of Si(100) using ion implantation. The C-rich Si and the Mn control are subsequently implanted at 300 °C with Mn ions, yielding a concentration profile of Mn (Mn%) ∼ 0.25 at. % within the depth of 160 nm. Post-implantation annealing is conducted in the range of 800-1000 °C. Ion channeling measurements suggest that Mn could occupy several lattice sites in Si including the tetrahedral interstitial and substitional site, with respective occupancy affected by carbon impurity and thermal annealing. The Hartree-Fock Cluster Method is used to calculate the binding energies of Mn for different lattice sites in Si. These structural information are compared with the results of superconducting quantum interference device (SQUID) experiments.

4:18PM D19.00008 Thermal Stability and Laser Annealing of Si1-fyCf alloys, STEFAN ZOLLNER, P. GRUDOWSKI, V. DHANDAPANI, G. SPENCER, A. THEAN, Freescale Semiconductor, Inc. — Dilute alloys of silicon and carbon are metastable, but can be produced (up to 3% C) using nonequilibrium growth techniques, such as chemical vapor deposition. In such alloys, carbon atoms are located at lattice sites (preferred for device applications) or at interstitial sites. Other impurities (such as H) can be introduced during the growth process. Since Si:C alloys are metastable, they usually do not survive typical source-drain dopant activation anneals (on the order of 1000°C for S). Also, Si:C alloys implanted with NMOS dopants do not recover as Si:C from ion implantation followed by pulsed laser melting and rapid solidification. We observed broadband subthreshold conduction below to a noisy, subthreshold (perhaps even percolative) path at lower voltages, with a significant contribution from the high density of defects at ∼5 V above the standard extrapolated threshold voltage. This field oxide structure has a length of 5 µm. We find that this variation is due to a transition from noisy subthreshold conduction to full conduction in strong inversion at a point that is more than ∼1 ms near the melting point), leading to an increase in the measured substitutional carbon content. This indicates a conversion of interstitial carbon defects into substitutional carbon or an evolution of hydrogen. We describe our results using a multiscale model applicable to thermal processing over a broad range of temperature and anneal times. Our model describes both solid-state regrowth and the loss or gain of substitutional carbon after annealing. We also present NMOS transistor results, where embedded Si:C alloy source-drain stressors lead to a reduction in the channel resistance.

4:30PM D19.00009 Chalcogen dopants for infrared optoelectronic Si, JEFFREY WARRENBERGER, US Army Benet Laboratories, BRION BOB, MICHAEL AZIZ, Harvard School of Engineering and Applied Sciences, SUPAKIT CHARNVANICHBORIKARN, JAMES WILLIAMS, Australian National University, MALEK TABBAL, American University of Beirut, ATSUSHI KOHNO, Fukuoka University — Doping Si with a chalcogen in excess of the solubility limit has been shown to result in subbandgap optical absorption and sensitive photodetection, suggesting potential for chalcogen-doped Si as an infrared optoelectronic material. We investigated optical absorption and photovoltaic energy conversion using S, Se, and Te as dopants. We achieved significant conversion efficiencies at extreme doping levels. We observed a gate-voltage dependence of the photovoltaic conversion efficiency for all dopants over a wavelength range from 1 to 2.3 microns. The subbandgap absorption and photovoltaic response depended sensitively on the chalcogen dose, laser processing, and thermal annealing conditions. We correlate these observations with the corresponding influence of the processing conditions on the material’s crystalline quality, chalcogen dopant depth profile, carrier concentration profile, and dopant activation. We found good agreement between the chalcogen depth profiles obtained from experiments and 1-dimensional model for plane-front melting, solidification, liquid-phase diffusion, and kinetic solute trapping.

4:42PM D19.00010 H-shuttling within a Hf-defect complex in Si/SiO2/HfO2 structures, A.G. MARINOPoulos, I. BATYREV, X. ZHOU, R. SCHRIMPF, D. FLEETWOOD, S.T. PANTELIDES, Vanderbilt University, Department of Physics and Astronomy — It was recently shown that, following irradiation of Si/SiO2/HfO2 structures by X-rays or constant-voltage stress, both oxide- and interface-trap densities exhibit oscillations with switch-bias annealing that are much larger than those previously observed in Si/SiO2 devices. Here we describe a particular defect complex that can account for the observations. The complex comprises a suboxide Hf-Si bond and an interfacial dangling bond (P center). With the aid of first-principles calculations we show that this defect possesses a symmetric double-well minimum and can provide trapping sites for H atoms near the interface. In the first site, the H atom passivates the dangling bond; in the second site the H atom resides near the center of the Hf-Si bond. A moderate intervening barrier (1.2 eV) suggests a relatively easy hopping of H atoms between these two energy minima, aided by the applied field and temperature. This shuffling mechanism can explain the observed oscillations in the interface trap densities during switched-bias conditions. This work was supported in part by the AFOSR and the DOE.

5:04PM D19.00011 Transition from high to low 1/f noise regimes in Field Oxide Field Effect Transistors (FOXFETs), XING ZHOU, DANIEL FLEETWOOD, RONALD SCHRIMPF, Vanderbilt University, LAURA GONELLA, FEDERICO FACCIO, CERN, PH Department, VANDERBILT COLLABORATION, CERN COLLABORATION — The excess low frequency (1/f) noise of parasitic field oxide FET (FOX) transistors from a 130 nm technology has been found to vary by more than ∼6 orders of magnitude with gate voltage, above the nominally measured device threshold. We find that this variation is due to a transition from noisy subthreshold conduction to full conduction in strong inversion at a point that is more than 5 V above the standard extrapolated threshold voltage. This field oxide structure has a length of ∼1 micron and a width of ∼200 micron. We attribute the conduction band modification to a substitution or interstitial carbon impurity at lower voltages, with a significant contribution from the high density of defects at ∼5 V above the Si/SiO2 interface in this parasitic FOXFET structure. The noise above the True threshold (as determined with assistance from the noise measurements) follows a standard number fluctuation model, when the subthreshold conduction regime is separated out in the analysis. This work was supported in part by the US Navy.

5:06PM D19.00012 Effects of Aging and Humidity on Low-Frequency Noise of Metal-Oxide-Semiconductor (MOS) Transistors, ARITRA DASGUPTA, Department of Physics & Astronomy, S.A. FRANCIS, Department of Electrical Engineering and Computer Science, D.M. FLEETWOOD, Department of Electrical Engineering and Computer Science, Vanderbilt University — Low frequency noise measurements can provide a non-destructive method of measuring radiation hardness and/or reliability of MOS transistors. We have been studying the effects of moisture exposure at elevated temperatures on MOS low frequency noise. The devices under test were manufactured in the 1980s and came from two different process lots. The results show that the normalized 1/f noise magnitudes K of the pMOS transistors increased significantly with exposure to humidity at elevated temperatures, while the changes in the 1/f noise magnitudes of the nMOS transistors were mostly much less. To estimate the energy dependence of the defects responsible for the noise, we evaluated the gate voltage dependence (Vg-Vt) of the noise, where Vt is the threshold voltage. We find, for the pMOS transistors, Snd−(Vg-Vt)−1, whereas, for the humidity exposed nMOS transistors, Snd−(Vg-Vt)−1.25. These deviations from an inverse square voltage dependence indicate a strong energy dependence of the defect distribution due to humidity exposure.

5:18PM D19.00013 Disorder–recrystallization effects following low-energy beam–solid interactions, MATTHEW J. BECK, Physics and Astronomy, Vanderbilt University, D. M. FLEETWOOD, R. D. SCHRIMPF, Electrical Engineering, Vanderbilt University, S. T. PANTELIDES, Physics and Astronomy, Vanderbilt University — Classical MD simulations have shown that thermal-spike-related disorder, including local melting, should be widely expected following high energy (>1 keV) recoils resulting from beam– solid interactions during ion-beam processing. In contrast, the formation of isolated point defects by direct atomic displacement is expected for low energy (<1 keV) recoils. Using state-of-the-art dynamical DFT calculations of Si–Si systems we show that recoils of much less than 1 keV result in highly disordered regions which persist for 100s of fs. Therefore, the production of beam-induced defects, as well as the post-implant yield of active dopants, following low-energy beam–solid interactions is controlled by dynamic recrystallization processes. This work was supported in part by the AFOSR through a MURI grant.
2:30PM D20.00001 Silicon Nanomembranes1. MAX G. LAGALLY, University of Wisconsin-Madison — Silicon nanomembranes (SiNMs) are extremely flexible, strain-engineered, defect-free, thin single-crystal sheets, with thicknesses from several 100 nm to less than 10 nm. Their novelty is several-fold: they are flexible, they are readily transferable to other hosts and conform and bond easily, they are stackable, and they can take on a large range of shapes (tubes, spirals, ribbons, wires) by engineering the strain and patterning the geometry. One can thus think of SiNMs as having inexact and tunable dimensionality, from 3-D to 0-D (when growth of quantum dots is included). Many properties of bulk Si are modified by thinness, strain, shape, and size, including band structure and quantum properties, electronic transport, phonon distributions, and mechanical properties. Because they are so close, the two surfaces of the membrane can influence each other’s behavior, and the surface also becomes a significant influence on overall SiN properties. After a review of SiNM fabrication, strain engineering, and transfer, we overview some of the unexpected physical and electronic properties of SiNMs. These include surface transfer doping via surface structures or adsorbed layers, through-membrane elastic interactions to create periodic strain lattices, energy level splitting and shifting with strain and quantum size effects, and orientation-dependent mobility enhancement with strain. SiNMs provide the potential for new or enhanced application of Si in fast flexible electronics; quantum electronics, new nanophotonic, optoelectronic, and thermoelectric devices; and chemical and biological sensors. These applications will be briefly outlined.

1Research supported by DOE, AFOSR, and NSF.

3:06PM D20.00002 Controlled displacement of nanoscale structures using an electron wind force. C.G. TAO, W.G. CULLEN, E.D. WILLIAMS, University of Maryland, College Park — Electromigration is widely used to drive mass transfer in the fabrication of nanogaps, and will be a crucial issue for the structural stability, reliability and performance of nanoscale electronic devices. Using a combination of scanning tunneling microscopy and scanning electron microscopy, we directly observe the biased motion of monatomic islands driven by the electron wind force on patterned single-crystal Ag(111) thin films. The island motion can be steered by changing the direction of the applied electric current. For monatomic adatom islands, the biased motion is opposite to the current direction and along the wind force direction, while vacancy islands move in the opposite direction. The measured dependence of the drift velocity on the island size, yields the product of the diffusion constant and the magnitude of the wind force, giving the diffusion constant $D = 1.56 \times 10^{10} \text{cm}^2/\text{s}$ for an effective charge of $e_s = 360 [1]$. The wind force acts even more strongly on Cu-decorated Ag(111) single-crystal pillars, as observed by directionally-oriented bending of step edges. The wind force needed to cause the observed structure distortions is $F = 0.13 \text{meV/\text{nm}}$, about 3 times the corresponding wind force acting on the bare steps. [1] A. Bondarchuk, et al. PRL 99, 206801 (2007).

1Work supported by the UMD NSF-MRSEC grant DMR 05-20471.

3:18PM D20.00003 Lateral alloy segregation in thin heteroepitaxial films. CHRISTIAN RATSCH, JASON REICH, XIAOBIN NIU, YOUNGJU LEE, RUSSEL CAFLISCH, UCLA — We have studied the segregation and alloy formation of thin heteroepitaxial films. We use an atomistic strain model that has a cubic geometry and includes nearest neighbor bonds, next nearest neighbor bonds, and bond bending terms. Our motivation is the well established fact that for many heteroepitaxial systems growth proceeds in the Stranski-Krastanov growth mode, where islands form after the formation of a wetting layer. Recent results indicate that intermixing and thus vertical variations of the alloy concentration are a crucial factor in controlling the formation and thickness of the wetting layer. Our results suggest that in addition to vertical segregation there is also lateral segregation. Thermodynamically, the system prefers to have one big feature of the epilayer material that is embedded in the substrate but is near the surface. In practise, there will be a typical separation distance of these features because of kinetic limitations. We postulate that this lateral segregation and the separation of these features is ultimately responsible for the lateral placement of islands on the surface.

3:30PM D20.00004 Two Species Diffusion Model of Self-Organized Evolution on Patterned GaAs(001) Surfaces*. HUNG-CHIH KAN, National Chung Cheng University, Taiwan ROC, ERIN FLANAGAN, TABASSOM TADAYYON-ESLAMI, University of Maryland, SUBRAMANIAM KANAKARAJU, Lab for Physical Sciences, CHRIS RICHARDSON1, RAY PHANEUF, University of Maryland — We report on numerical simulations of the self-organized evolution on GaAs(001) surface, pre-patterned with square arrays of pillars, during homo-epitaxial growth. Our experiments showed that lithographically fabricated, flat-topped cylindrical pillars evolved into a universal, downward paraboloidal shape, for initial diameters of the pillar ranging from 0.7um to several microns. In modeling this behavior, we construct a two-species diffusion model to simulate the growth. We use an atomistic strain model that has a cubic geometry and includes nearest neighbor bonds, next nearest neighbor bonds, and bond bending terms. Our motivation is the well established fact that for many heteroepitaxial systems growth proceeds in the Stranski-Krastanov growth mode, where islands form after the formation of a wetting layer. Recent results indicate that intermixing and thus vertical variations of the alloy concentration are a crucial factor in controlling the formation and thickness of the wetting layer. Our results suggest that in addition to vertical segregation there is also lateral segregation. Thermodynamically, the system prefers to have one big feature of the epilayer material that is embedded in the substrate but is near the surface. In practise, there will be a typical separation distance of these features because of kinetic limitations. We postulate that this lateral segregation and the separation of these features is ultimately responsible for the lateral placement of islands on the surface.

*supported by the Lab for Physical Sciences and by NSF# DMR-0705447.

3:42PM D20.00005 Directed Matrix Seeding of Nitride Semiconductor Nanocrystals. A.W. WOOD, B.L. CARDOZO, W. YE, X. WENG, R.S. GOLDMAN, Materials Science and Engineering, Univ. of Michigan, Y.Q. WANG, Materials Science and Tech. Division, LANL — The controlled formation of semiconductor nanocomposites offers a unique opportunity to tailor functional materials with a variety of novel properties. A promising approach to nanocomposite synthesis is matrix-seeded growth, which involves ion-beam-amorphization of a semiconductor film, followed by nanoscale re-crystallization via annealing. In this work, we are studying the formation and evolution of N-ion-implanted InAs and GaAs (InAs:N, GaAs:N). The InAs:N and GaAs:N nanocomposites are synthesized using 100keV ion-implantation with a dose of $5\times10^{15}/cm^2$ for an effective charge of $z_s = 360 [1]$. The wind force acts even more strongly on Cu-decorated Ag(111) single-crystal pillars, as observed by directionally-oriented bending of step edges. The wind force needed to cause the observed structure distortions is $F = 0.13 \text{meV/\text{nm}}$, about 3 times the corresponding wind force acting on the bare steps. [1] A. Bondarchuk, et al. PRL 99, 206801 (2007).

1Lab for Physical Sciences
3:54PM D20.00006 Nanofabrication of carbon materials, DINKO CHAKAROV, HANS FREDRIKSSON, BENGT KASEMO, Chalmers University of Technology. DEPARTMENT OF APPLIED PHYSICS TEAM — We demonstrate a process for fabrication of nanostructures on the surfaces of highly oriented pyrolytic graphite (HOPG) and glassy carbon (GC) samples. Using hole-mask colloidal lithography (HCL), nanosized etch masks with three different feature diameters were prepared by identical processes on each of the two surface types. Oxygen reactive ion etching (RIE) was then used to transfer the mask pattern onto the surfaces. The structures were characterized using atomic force- (AFM), scanning electron microscopy (SEM) and optical spectrophotometry. The identical preparation schemes applied to the two materials yield structures with remarkably different shape and sizes. For example the process that yields 361 nm high and 37 nm diameter structures on glassy carbon yields 120 nm high and 119 nm diameter structures on HOPG. In general, the diameters of the fabricated GC nano-features are always at least 80 nm smaller than those of the corresponding HOPG structures, and the GC structure heights are more than three times that of the HOPG structures. These differences are attributed to different (an)isotropic etching behavior of the two materials.

4:06PM D20.00007 Fabrication of Metallic Nanoporous Films by Selective Chemical Etching, SHILPA CHAVA, WEI JIANG YEH, University of Idaho — The objective of this study is to synthesize and characterize different nanoporous structures by chemical etching. The experiments were conducted on three different materials. We treated 6 carat white gold (Au/Au alloy, 1:3 ratio by weight) with 70% HNO3 to grow Au nanoporous, the 50/50 solder wire (Pb/Sn alloy) with 93% H2SO4 to create Pb porous and Imitation Italian gold leaf (Cu/Zn alloy, 82/18 by wt. %) with NaOH solution (5 gm NaOH per 100 ml distilled H2O) for Cu porous. The free-standing porous films have been analyzed by scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDX), high quality x-ray mapping (XRM). We observed the composition of the porous materials at every stage of chemical dealloying and conducted tests with different process parameters to optimize the size of self-ordered porous structures. Our experiments resulted in sponge like Au nanoporous of 10-200 nm, Pb pores of 10-300 nm and Cu pores of 10-150 nm. The results showed a technically improved fabrication of different nanoporous materials with high surface area and well defined pore morphology.

4:18PM D20.00008 Formation of Periodic 2D Metallic Nanostructures by Template-Assisted Electrodeposition, MU WANG, BO ZHANG, YUYAN WENG, RUWEN PENG, NAIBEN MING, Department of Physics, Nanjing University, Nanjing 210093, China — Two-dimensional ordered metallic nanostructures on solid surface with specific patterns may have potential applications in photonics and optoelectronics. Yet it remains a challenge to produce regular nanostructures over a large area with low cost and with a simple method. Here we report a novel method to fabricate well-aligned copper nanowire array on silicon surface by template-assisted electrodeposition. The template is introduced onto silicon surface by nanoimprinting. With our previously reported unique electrodeposition system [1-2], we find that the array of straight copper wires with their width varying from 400 nm to 20 nm can be fabricated. The wire width can be tuned by the control parameters in electrodeposition. It is shown that this method is not limited to straight wires only. It can be used to form more complicated patterns. The physical properties of the metallic nanostructures are also discussed. [1]


4:42PM D20.00010 Fabrication of High-Aspect-Ratio Nanogaps, ALEXANDRA FURSINA, Department of Chemistry, Rice University, 6100 Main St., Houston, TX 77005, SUNGBAE LEE, Department of Physics and Astronomy, Rice University, 6100 Main St., Houston, TX 77005, DOUGLAS NATelson, Department of Physics and Astronomy, Department of Electrical and Computer Engineering, Rice University, 6100 Main St., Houston, TX 77005 — For nanoscale electrical characterization and device fabrication it is often desirable to fabricate planar metal electrodes with separations well below 100 nm running parallel over a macroscopic width. In this work we demonstrate a self-aligned process to accomplish this goal using a thin Cr film as a sacrificial etch layer. The resulting gaps can be as small as 10 nm and have aspect ratios exceeding 1000, with excellent interelectrode isolation. Two separate lithographic patterning steps are used to define first and second electrodes while the interelectrode separation is controlled by the oxidation of a Cr layer deposited upon the first electrode. Advantageously, only a µm-alignment of first and second electrodes is required and the described method effectively does not have limitations on the gap width while the length of the gap is controlled by the Cr layer thickness. In addition to fabrication of Ti/Au electrodes on Si substrates, our technique was also demonstrated to work for other electrode metals (Pt, Fe, etc.) even on such relatively reactive substrates as magnetite, F3O4, films, thus demonstrating the flexibility and utility of this method.

4:54PM D20.00011 Subtle role played by H in Si thin-film growth from radicals: key atomic-scale mechanisms revealed by DFT calculations, F. MONTALENTI, S. CEREDA, LEO MIGLIO, F. ZIPOLI, M. BERNASCONI, L-NESS and Materials Science Department, University of Milano-Bicocca, Milan (Italy), M. CERIOTTI, Department of Chemistry and Applied Biosciences, ETH Zurich — Breaking silane molecules and creating reactive radicals in the gas phase is an efficient strategy for growing Si films at high growth rates and/or moderate temperatures. In a seminal experimental paper [1], the possibility of obtaining crystalline growth down to T~200°C, was clearly demonstrated under high dilution of radicals in H. Several interpretations, in some cases controversial, have been given for explaining this evidence. Here we shall show that a clear understanding can be reached by relying on DFT calculations. Starting by a fully hydrogenated Si(001)(1×2) surface, typical of low-temperature growth, we first illustrate the role played by SiH3 in removing adsorbed H, therefore creating empty sites for further SiH3 adsorption [2]. The adsorbed silyl, however, is frozen in its initial, non-epitaxial configuration, so that crystalline growth cannot take place. We demonstrate that further incoming hydrogen can easily transform silyl into SiH2, which, in turn, incorporates into epilayer sites crossing a barrier of only ~1 eV [3], compatible with Ref. [1] conditions. [1] C.C. Tsai et al., J. Non-Cryst. Solids 114, 151 (1989). [2] S. Cereda et al., Phys. Rev. B 75, 235311 (2007), Phys. Rev. Lett. (in press).
transition metal atoms substituting for Zn atoms within the cage.

Our studies are carried out within a density functional framework employing gradient corrected functionals. The studies cover all the 3d elements and examine the strength of the magnetic moment as substituting Zn atoms by transition metal atoms or by encapsulating transition metal clusters inside the cages. Our studies are carried out within a density functional framework.

Films, SUMEET PANDEY, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report results from kinetic Monte Carlo simulations of plasma deposition of silicon thin films under conditions that render the SiH₄ radical the dominant deposition precursor. The transition probabilities for the various kinetic events accounted for in the simulations are based on first-principles density functional theory (DFT) calculations of the corresponding optimal pathways on the H-terminated Si(001)-(2×1) surface and on molecular-dynamics simulations on hydrogenated amorphous silicon film surfaces. The relevant surface transport and reaction processes include SiH₄ diffusion, SiH₄ chemisorption and insertion into Si-Si bonds, surface H abstraction reactions, surface hydride dissociation reactions, as well as SiH₄ and SiH₂ desorption into the gas phase. Surface etching is predominantly observed over the 373-640 K temperature range. The surface compositions obtained are in good agreement with experimental measurements on films deposited under similar growth conditions. At 500 K, surface SiH₂ formed by surface trihydride dissociation reactions is the dominant surface hydride species.

Isotopic interfaces in a structurally anisotropic organic thin film ¹, C. G. TAO ², Q. LIU, B. RIDDICK, W. G. CULLEN, D. EVANS, J. REUTT-ROBEY, J. D. WEEKS, E. D. WILLIAMS, University of Maryland — We investigate the interfacial boundary fluctuations of Acridine-9-Carboxylic Acid (ACA) deposited on Ag(111) using UHV STM. The ACA molecule is anisotropic in shape and intermolecular interactions, and has been shown to exhibit a disordered 2D gas phase on Ag(111) at low coverage. At higher coverage, the molecules arrange in domains of ordered chain-like structures which coexist with the disordered phase. We measure the real-time fluctuations at the phase boundaries, and show that these fluctuations are governed by molecular exchange between the two phases. Due to structural anisotropy, there are two types of domain boundaries with significantly different molecular interactions. Surprisingly, the fluctuation magnitudes, mobilities, and free energies are nearly equal for the two boundary types. A lattice-gas statistical model is presented which includes the influence of molecular conformations on substrate interactions, and reproduces the essential features observed experimentally: domain shapes, boundary fluctuations, and phase densities.

Supports from US AFOSR, ARO and DOE

From Designer Clusters to Synthetic Crystalline Nano-Assemblies ¹, MEICHUN QIAN, S. KHANNA, A. REBER, Dept. of Physics, Virginia Common. Univ., A. CASTLEMAN, A. SEN, A. UGRINOV, K. DAVIS, S. PEPPERNICK, M. MERRITT, Dept. of Chemistry and Physics, Penn. State Univ. — Clusters have the potential to serve as building blocks of materials, enabling the tailoring of materials with novel properties. We have recently proposed a new protocol that combines gas phase investigations to examine feasible units, theoretical investigations of energy landscapes to identify potential motifs, and synthetic chemical approaches to synthesize cluster assemblies. We had earlier applied the protocol to As₃− clusters based cluster assemblies. In this work, we extend our investigations to cluster assembled materials based on As₁₃− units as building blocks. By varying the alkali cation and introducing crypts, it is possible to form materials with arsenic clusters arranged to form one dimensional chains, two dimensional layers or three dimensional lattices and X-ray studies provide information on bond lengths etc. Theoretical studies have been carried out to examine their microscopic structure and electronic properties. It will be shown that these new compounds have the tunable electronic and optical properties. The theoretical predictions on the As₁₃− Crypt(Κ) and [As₁₃−Cs₂]¹− Crypt(Κ) are in good agreement with the experimental observations.

Geometries and stabilities of Ag-doped Siₙ (n = 1 - 13) clusters: a first-principles study ¹, FENG-CHUAN CHUANG, YUN-YI HSIEH, CHIH-CHIANG HSU, MARVIN ALBAO, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The structures of AgSiₙ (n = 1 - 13) clusters are investigated using first-principles calculations. Our studies suggest that AgSiₙ clusters with n = 7, and 10 are relatively stable isomers and that these clusters prefer to be exohedral rather than endohedral. Moreover, doping leaves the inner core structure of the clusters largely intact. Additionally, the plot of fragmentation energies as a function of silicon atoms shows that the AgSiₙ are favored to dissociate into one Ag atom and Siₙ clusters. Alternative pathways exist for n > 7 (except n = 11) in which the Ag-Si cluster dissociate into a stable Siₙ and a small fragment Agₙ−7. The Agₙ−7 cluster dissociates into a stable Siₙ−3 and a small fragment Agₙ−10. Lastly, our analysis indicate that doping of Ag atom significantly decreases the gaps between the highest occupied molecular orbital and the lowest unoccupied molecular orbital for n > 7. Reference: J. Chem. Phys. 127, 144313 (2007).

Transition Metal Doped and Encapsulated ZnO Cages, MARCELA R. BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, ARTHUR REBER, SHIV N. KHANNA, Physics Department, Virginia Commonwealth University — ZnO is a wide band gap semiconductor with potential for applications. We had earlier shown that Zn₁₂O₁₂, Zn₁₅O₁₅, Zn₁₈O₂₈, and Zn₂₁O₂₃ clusters are particularly stable and exhibit cage structures. In this work, we examine the possibility of making magnetic materials by either substituting Zn atoms by transition metal atoms or by encapsulating transition metal clusters inside the cages. Our studies are carried out within a density functional framework employing gradient corrected functionals. The studies cover all the 3d elements and examine the strength of the magnetic moment as well as the nature of the coupling between the local moments. We also present results on the coupling between the endohedral transition metal cluster and the transition metal atoms substituting for Zn atoms within the cage.
3:42PM D21.00005 DFT study of a carotenoid-porphyrin-C_{60} light-harvesting molecular triad
TUNA BARUAH, University of Texas at El Paso — The abundance of solar energy reaching the earth presents an attractive alternative energy source. Nearly 75% of the solar energy striking the upper atmosphere reaches the earth in the form of photons of energy typically higher than 1 eV. Biological light-harvesting systems are highly efficient in utilizing the solar radiation. Bio-mimetic molecules are investigated to mimic the photosynthesis process efficiently in laboratory. We present a computational study of the process in a bio-mimetic carotenoid-porphyrin-C_{60} molecular triad which is about 5 nm long. The description of the photo-induced charge separation process requires accurate excited state energies and coupling between electrons and the phonons of the system. Since charge-transfer excitations create large changes in a molecular dipole moment, changes in excited-state energies due to coupling between a 5 nm molecular photovoltaic and the surroundings (solvent and spectator molecules) also has to be taken into account. A density functional theory based method including all these effects to describe the photo-induced charge separation process will be presented.
1ONR, UTEP, NSF

4:18PM D21.00006 Spin Accommodation and Reactivity of Superatoms
ARTHUR REBER, Virginia Commonwealth University — We have recently discovered novel effects that may allow tuning of the reactivity of small clusters by controlling their spin excitation, electronic structure, and local geometry. These findings offer the prospect of designing new catalysts through cluster assemblies where chosen clusters, called superatoms, serve as elemental building blocks. Taking aluminum as an example, I will present our recent findings that illustrate how reactive clusters can be made non-reactive while inert species can be made reactive by adding hydrogen atoms. These findings offer a microscopic understanding of the recent experimental reactivity studies on aluminum and aluminum-hydride clusters that show variable reactivity in even electron systems and rapid etching in odd electron systems. It is shown that the reactivity of even electron clusters is governed by a spin transfer, from the triplet oxygen to the cluster, that fills the spin down antibonding orbitals on oxygen. Theoretical investigations show that when the spin transfer cannot occur, the species is unreactive, and when spin accommodation is possible, more subtle effects appear. Secondly, I will examine the reactivity of aluminum clusters with simple nucleophiles such as water. The reactivity and nature of the ensuing products is wildly variable with the size and shape of the cluster. Again, the electronic structure and local coordination of the active sites allow for an understanding of changing barrier heights and resulting reactivity. This work provides a framework with which new catalysts may be designed.
11 gratefully acknowledge support from MURI grant W911NF-06-1-0280 and the Department of Energy (DE-FG02-06ER45579).

4:54PM D21.00007 Peierls distortion of endohedral atoms in clathrate I. HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University, Japan — The guest atom displacements in type II clathrates have been reported on experimental and theoretical points of view. The displacements are reported to be 0.6 Å from the cage center of the Si_{28} cage to the hexagonal in the hydrogen terminated double caged Si_{28} cluster [1]. The distortion can be expected to occur in the type I clathrate which forms with bamboo structures in the x, y, and z directions. The guest atoms show Peierls distortion when we calculate the equilibrium distances between the two Na atoms which locate at the neighboring Si_{28} cages in the bamboo structure using periodic density functional calculation. The binding energy between the guest atoms is −0.10 eV/Na_{2}. We also confirm the tendency of the Peierls distortion from the force directions of guest atoms in the double unit cells that contain four Na atoms in one dimension; We will propose the cohesion mechanism of the clathrates that the clathrates are precipitated states of the connecting endohedral atoms in the 14 group atoms. So are the hydroclathrates in which the guest molecules bind each other with chains. [1] H. Takenaka and K. Tsumuraya, Mater. Trans. 47, 63 (2006).

5:06PM D21.00008 [Te_{2}As_{2}]^{2−}: A Planar Motif with Potential for Ferromagnetism
SHIV KHANNA, ARTHUR REBER, MEICHUN QIAN, Virginia Commonwealth University, ANGEL UGRINOV, AYUSMAN SEN, Pennsylvania State University — Here we report the synthesis and crystal structure of [K(18-crown-6)][Te_{2}As_{2}], the first four-membered ring Zintl anion of elements from groups XV and XVI, isolated from an ethylenediamine solution of As, K, and As_{2}Te_{2} at room temperature. X-ray analysis indicates that the [Te_{2}As_{2}]^{2−} anion has an unexpected planar rhombic structure with alternating bonds. First-principles electronic structure investigations within the density functional framework, indicate that the Te_{2}As_{2}K_{2} motif possesses a triplet ground state where the spin configuration leads to a distortion of the square geometry into rhombus structure marked by two Te-As shorter bond length pairs joined by longer bond lengths. A NICS analysis reveals that the triplet motif has a net aromatic character. Supercell calculations on the periodic solid show that the spin moments on the individual motifs order ferromagnetically thus offering the potential of an aromatic ferromagnet made of traditionally non-magnetic elements.
1We gratefully acknowledge support from the U.S. Department of the Army through MURI grant W911NF-06-1-0280, Department of Energy (DE-FG02-96ER45579), and AFOSR (FA9550-05-1-0186).

Monday, March 10, 2008 2:30PM - 5:18PM –
Session D22 DMP DPOLY: Focus Session: Organic Electronics: Synthesis and Materials Morial Convention Center 214

2:30PM D22.00001 The role of symmetry and charge delocalization in two-dimensional molecules conjugated molecules for optoelectronic applications
MARY GALVIN — Our group is investigating whether star molecules offer any advantage over linear polymers when used as the active layer in light-emitting diodes (LEDs), organic transistors (OFETs) or in photovoltaics (PVs). Specifically, we are investigating the role of architecture, synthesizing some novel molecules that contain a central tetra substituted phenyl ring. These molecules have a tendency to pi-pi stack, further delocalizing the carriers. The synthetic strategy used to prepare these molecules is versatile so that the four arms in the molecules do not have to be identical. The placement of differing arms also affords the opportunity to study the effect of symmetry on the properties of these molecules. The HOMO and LUMO levels can be changed via the type and placement of arms. Recent results obtained with these materials and their applications in photovoltaics and light-emitting diodes will be described.
1The author thanks NSF for support of this work (DMR0513348).
3:06PM D22.00002 Ultra-pure organic semiconductors with improved charge carrier transport properties, CLARA SANTATO, Département de Génie Physique, École Polytechnique de Montréal, C.P. 6079, Succ. “Centre Ville”, Montréal, QC, Canada H3C 3A7, FABIO CICOIRA, Department of Material Science and Engineering, Cornell University, Ithaca, NY, 14853-1501 and INP - CNR Via alla Cascata 56c Povo (TN), 38050, Italy, FRANCESCA DI MARIA, MANUELA MELUCCI, GIOVANNA BARBARELLA, ISOF -CNR, Via P. Gobetti 101, 40129 Bologna, Italy — The electrical performance of devices based on organic semiconducting films depend critically on the synthesis and processing of the materials. The quality of organic semiconductors depends on synthetic conditions and purification procedures, which have not yet been optimized. Ultra-pure semiconductor materials are required to establish sound correlations between molecular structure, functional properties of the films and performance of devices based thereon, e.g. field-effect transistors (FETs). Understanding structure-property relationships in films is the crucial condition for predicting chemical structures with superior properties. We report on FETs based on oligothiophene that exhibit dramatically improved charge transport, due to the ultra-purity of the organic semiconductors. The latter was achieved using a synthetic methodology that takes advantage of (i) heterogeneous catalysts, (ii) microwave activation to shorten reaction times and suppress side reactions.

3:18PM D22.00003 Side Chain Structure and Density of Polymers in different Complex Fluids, YUNFEI JIANG, DVORA PERAHIA, Chemistry Department, Clemson University, Clemson, SC, 29634, YIQING WANG, UWE H. F. BUNZ, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332 — Pol (para phenyleneethynylene) (PPE) polymers are electro-optically active macromolecules with immense potential in organic electro-optical devices. The polymer backbones are substituted by side chains that affect their conformation, association modes and dynamics. Consequently, they modify the optical response of the polymer. The present work introduces a small angle neutron scattering (SANS) and neutron spin echo (NSE) measurement of PPE substituted with a bulky triisopropylsilyl (TIPS) side chain in toluene. The results are compared with those previously obtained results of alkyl substituted PPEs. While alkyl substituted PPEs interacts via pi-pi stacking and forms a fragile gel, TIPS-PPE associates predominantly via the side chains and forms a stable gel over a large temperature range. The dynamics of PPEs in gel includes both fast and slow components and a cooperative dynamics between the solvent and PPE molecules.

3:30PM D22.00004 Thermal, structural, and electrical characterization of two high performance semiconductor polymers, L.J. RICHTER, NIST, Gaithersburg, MD, A.J. MOAD, D.M. DELONGCHAMP, R.J. KLINE, D.J. GUNDLACH, D.A. FISCHER, NIST, I. MCCULLOCH, Imperial College, London, UK, M. HEENEY, Queen Mary University, London, UK — Polymer semiconductors are expensive solution processable polymers with minimal issues due to the presence of flexible large area electronics. Recently, thin films of spin-cast poly(2,5-bis(3-alkylthieno[3,2-b]thiophene)-2,5-bithiophene) (pTTBT) after heating into a mesophase. Poly(dialkylthiophene)[3,2-b]thiophene-2,5-bithiophene) (pTTBT) is a newly synthesized isomer of pTTBT with side chains attached to the thiophenothiophene rather than the bithiophene unit. This subtle structural change results in a very different response to heating. FTIR, spectroscopic ellipsometry (SE), AFM, X-ray diffraction, and NEXAFS were utilized to determine the root of the different thermal behavior. The structural transitions of the isomers are generally similar; however, the side chain melting transition T_m occurs about 50˚C lower in pTTBT than in pBTBT. The significant drop in T_m appears to correlate with a subtle decrease in main chain packing interactions. Both materials exhibit high hole mobility, even in their respective mesophases. The slight overall higher order in pBTBT is reflected in the device performance.

3:42PM D22.00005 Synthesis and characterization of conducting polymer inserted carbon nanotubes, A. JONG CHOI, YOUNG WOO NAM, YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University — The carbon nanotubes filled with the photo-conducting polymer poly(N-vinyl carbazole) (PVK) as a conducting polymer were prepared by polymerizing the monomers inside the nanotubes using the supercritical carbon dioxide. The endohedral nanotubes were characterized by HRTEM and 1H NMR, which confirmed that the inserted material was indeed the conducting polymer [1]. 1-V characteristics of the polymer inserted carbon nanotubes are presented. [1] Johannes Steinmetz, Soyoung Kwon, Hyun-Jung Lee, Eddy Abou-Hamad, Robert Almainac, Christophe Goze-Bac, Hwayong Kim, Yung-Woo Park., Chem. Phys. Lett. 431, 139 (2006)

3:54PM D22.00006 X-ray scattering Study of Ordering in Liquid Crystalline Semiconducting Polymers, MICHAEL CHABINYC, Palo Alto Research Center, MICHAEL TONEY, Stanford Synchrotron Research Laboratory, IAIN MCCULLOCH, Imperial College, MARTIN HEENEY, Queen Mary University of London — The electrical performance of thin-film transistors, TFTs, formed with semiconducting polymers is approaching that of amorphous silicon. The highest performance TFTs are obtained from semiconducting polymers with liquid crystalline (LC) mesophases. Thermal annealing of these materials after deposition can increase the field effect mobility by as much as an order of magnitude. We will report the results of detailed x-ray scattering studies of the impact of thermal annealing on the crystalline ordering in thin films of poly(2,5-bis(3-n-alkyl-2-yl)thieno[3,2-b]thiophene) (pTTBT). Poly(2,5-bis(3-n-alkyl-2-yl)thieno[3,2-b]thiophene) (pTTBT) is a newly synthesized isomer of pBTBT with side chains attached to the thiophenothiophene rather than the bithiophene unit. This subtle structural change results in a very different response to heating. FTIR, spectroscopic ellipsometry (SE), AFM, X-ray diffraction, and NEXAFS were utilized to determine the root of the different thermal behavior. The structural transitions of the isomers are generally similar; however, the side chain melting transition T_m occurs about 50˚C lower in pTTBT than in pBTBT. The significant drop in T_m appears to correlate with a subtle decrease in main chain packing interactions. Both materials exhibit high hole mobility, even in their respective mesophases. The slight overall higher order in pBTBT is reflected in the device performance.

4:06PM D22.00007 Improving the Electrical Conductivity of Polyaniline Through Molecular and Structural Control, JOYOUNG EUN YOO, Princeton University, University of Texas at Austin, YUEH-LIN LOO, Princeton University — We have investigated the electrical conductivity of polyaniline (PANI) that is template synthesized with a polymer acid of poly(2-acrylamino-2-methyl-1-propanesulfonic acid), PAAMPSA, as a function of the polymer acid molecular characteristics, including its molecular weight and molecular weight distribution. The electrical conductivity of PANI-PAAMPSA increases with decreasing PAAMPSA molecular weight. PANI that is doped with narrow molecular weight distribution PAAMPSA is twice as conductive as PANI that is doped with PAAMPSA of molecular weight and molecular weight distribution. In this case, the conductivity of PANI-PAAMPSA improves by more than two orders of magnitude. UV-vis-NIR spectroscopy and X-ray photoelectron spectroscopy suggest that DCA suppress side reactions.

4:18PM D22.00008 Surface photoisomerization activity vs. functionalization of azobenzene derivatives, LUIS BERBIL-BAUTISTA, JONGWON CHO, NIV LEVY, MATTHEW J. COMSTOCK, DAN POULSEN, JEAN M.J. FRECHET, MICHAEL F. CROMMIE, University of California at Berkeley — Azobenzene and its derivatives can be reversibly photoisomerized between their cis and trans conformations in solution. The photoisomerization process is wavelength selective and results in a large length change. Hence, it is ideally suited to actuating molecular nanomachines on surfaces. However, it has recently been shown [1] that photoisomerization activity on a metallic surface must be functionalized with bulky spacing groups to decouple the optically active part of the molecule from the surface. This results in various trade-offs between molecular optical activity and overall flexibility/functionality. We have explored the photoisomerization activity of different azobenzene derivatives on metallic surfaces using a scanning tunneling microscope (STM) with optical access to the sample. The effects on molecular photo-activity and self-assembly for different substitutional groups has been studied. [1] Matthew J. Comstock, Niv Levy, Armen Kirakosian, Jongweon Cho, Frank Lauterwasser, Jessica H. Harvey, David A. Strubbe, Jean M. J. Frechet, Dirk Trauner, Steven G. Louie, and Michael F. Crommie Phys. Rev. Lett. 99, 038301 (2007)
4:30PM D22.00009 Electrical and Optical Properties of a Novel Nonconjugated Conductive Polymer, Polynorbornene, ANANTHAKRISHNAN NARAYANAN, ADITYA KUMAR PALTII, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — We report electrical and optical properties of a novel nonconjugated conductive polymer, polynorbornene which has an isolated double bond in the repeat. Electrical conductivity of this polymer increases by more than ten orders of magnitude to about 0.01 S/cm upon doping with iodine. Optical absorption measurements of the polymer film have been made at different dopant concentrations. For a lightly doped polymer, two absorption peaks: one corresponding to cation radicals and the other corresponding to charge transfer between the double bond and the dopant were observed at 4.20 eV (295nm) and 3.13 eV (396nm) respectively. FTIR spectroscopic measurements have shown a reduction in the intensity of the C=C stretching and C-H bending vibration bands upon doping indicating formation of radical cations. Photoluminescence studies have shown an emission band with a peak at ~425nm when excited at 300nm. Nonlinear optical studies of this novel nonconjugated conductive polymer are in progress.

4:42PM D22.00010 Quadratic Electro-optic Measurements in the Nonconjugated Conductive Polymer, Poly(β-pinene) at 800 nm and 1550 nm, JITTO TITUS, ANANTHAKRISHNAN NARAYANAN, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — Electro-optic effect in the nonconjugated conductive polymer, iodine-doped poly(β-pinene) measured at 633 nm has been recently reported. In this presentation, results of quadratic electro-optic measurements at longer wavelengths will be reported. The electro-optic measurement has been made using the field-induced birefringence technique in the cross-polarized geometry with lock-in detection. Films with a medium doping level of iodine have been used in the measurements. Modulation depths of about 1.1% at 800 nm and 0.06% at 1550 nm were observed for an applied ac field of about 1 Volt/µm and for a film thickness of about 1 µm. More detailed measurements are in progress. The results are highly promising for applications of these materials in electro-optic modulators in the channel waveguide configuration. This exceptionally large quadratic electro-optic effect has been attributed to the confinement of this electronic system within a sub-nanometer dimension and the special electronic structure of this doped system.

5:06PM D22.00012 Direct Nanoscale Characterization of Submolecular Mobility in Complex Organic Non-linear Optical Systems, DANIEL KNORR, TOMOKO GRAY, TAE-DONG KIM, JINGDONG LOU, ALEX JEN, RENE OVERNEY — For organic non-linear optical (NLO) materials composed of intricate molecular building blocks, the challenge is to deduce meaningful molecular scale mobility information to understand complex relaxation and phase behavior. This is crucial, as the process of achieving a robust acenctic alignment strongly depends on the availability of inter- and intra-molecular mobilities outside the temperature range of the device operation window. Here, we introduce a nanoscale methodology based on scanning probe microscopy that provides direct insight into structural relaxations and shows great potential to direct material design of sophisticated macromolecules. It also offers a means by which mesoscale dynamics and cooperativity involved in relaxation processes can be quantified in terms of dynamic entropy and enthalpy. This study demonstrates this methodology to describe the mesoscale dynamics of two systems (1) organic networking dendronized NLO molecular glasses that self-assemble into physically linked polymers due to quadrupolar phenyl-perfluorophenyl interactions and (2) dendronized side-chain electro-optic (EO) polymers. For the self assembling glasses, the degree of intermolecular cooperativity can be deduced using this methodology, while for the dendronized side-chain polymers, specific side chain mobilities are exploited to improve EO properties.

Monday, March 10, 2008 2:30PM - 5:30PM —
Session D23 DMP GMAG: Focus Session: Triangular Lattice and Spinels Morial Convention Center 215

2:30PM D23.00001 Magnetic ordering and structural transition in layered Li$_2$RuO$_3$1, DEVINA PILLAY, MICHELLE JOHANNES, Naval Research Laboratory — Li$_2$RuO$_3$ is a layered, triangular-lattice metal oxide system much like Na$_2$CoO$_2$, NaNiO$_2$ and LiNiO$_3$ with the exception that one of every three transition metal ions (Ru) is replaced by a Li ion. This results in a honeycomb arrangement of spin-carrying ions and eliminates the magnetic frustration intrinsic to the triangular lattice. Here we investigate the electronic structure of Li$_2$RuO$_3$, especially in relation to its magnetic ordering both in-plane and between adjacent planes. We find that the dimerization of Ru atoms within the metal-oxide planes acts in conjunction with magnetic ordering to establish a gapped, magnetic ground state. The change in the energy level spectrum brought on by the formation of spin-polarized Ru-Ru molecular orbitals replaces the expected Jahn-Teller mechanism as a way of relieving a degeneracy at the Fermi energy.

1Fundied by the Office of Naval Research. DP is funded by the National Research Council.

2:42PM D23.00002 Magnetic interactions in geometrically frustrated triangular lattice antiferromagnet CuFeO$_2$, JAIME FERNANDEZ-BACA, FENG YE, RANDY FISHMAN, ORNL, H. J. KANG, J. W. LYN, NIST, TSUYOSHI KIMURA, Osaka University — Geometrically frustrated magnetic systems have received considerable attention due to their extraordinary magnetic properties. The delafossite CuFeO$_2$ is of particular interest because it exhibits multiferroic behavior with either the application of a magnetic field or introduction of nonmagnetic impurities. Our recent [1] on CuFeO$_2$ shows that spin waves in this material can be explained by antiferromagnetic interactions up to third nearest neighbors within the hexagonal plane as well as out-of-plane coupling, indicating that the quasi-like fising nature of this material results from the delicate balance between competing interactions. Two energy dips in the spin dispersion occur at the incommensurate wavevectors associated with multiferroic phase, and are dynamic precursors to the magnetoelectric behavior. In this talk we will present preliminary measurements of the field magnetic field dependence of these excitations as CuFeO$_2$ approaches the multiferroic phase [1] Ye et al. Phys. Rev. Lett. 99, 157201 (2007)
The change in properties has been understood in terms of site preference of the dopant cation. The current study investigated the temperature dependence and GaN.

The results confirm the existence of two phase transitions. The first, near 56 K, is from a paramagnetic state to a collinear ferrimagnetic phase. There is a second simultaneous structural and magnetic transition at 53 K to a tetragonal structure with a non-collinear ferrimagnetic state. The low-temperature magnetic structure has been definitively resolved, and is seen to be associated with a gap in the magnetic excitation spectrum. The magnetic structure is compatible with a staggered orbital ordering. Inelastic scattering has been carried out using both triple axis and time of flight techniques, and several branches of magnetic excitations are visible. These observations put tight constraints on theoretical models for MnV

NIST Center for Neutron Research, CHRIS FROST, Rutherford-Appleton Laboratories — Neutron diffraction and inelastic scattering has been used to study the Magnetic and magnetoelastic properties of Ge-substituted cobalt ferrite.

Neutron Scattering Study of Magnetic and Orbital Order in MnV₂O₄.

We discuss the changes in ground states as a function of Lithium content, and we review magnetic and magnetoelastic properties of germanium substituted cobalt ferrite, C₀₁₋ₓGe₂Fe₂₋ₓO₄, over a temperature range of 10 – 400 K. Both magnetic hysteresis loops and magnetostriction loops have been measured for several selected compositions with 0 ≤ x ≤ 0.8. At room temperature, saturation magnetization, magnetic anisotropy and magnetostriction were seen to decrease with increasing Ge-content. This new class of materials is therefore highly suitable for magnetic sensor and actuator applications in which the magnetic properties can be tailored to meet specific needs.

Charge order and frustrated magnetism in the orbitally-degenerate triangular metallic antiferromagnet AgNiO₂. RADU COLDEA, University of Bristol, UK — We explore the electronic ground state in the orbitally degenerate triangular metallic antiferromagnet AgNiO₂. In high-resolution neutron diffraction we observe a structural transition below 365 K to a trilayer unit cell in the triangular layers with a periodic arrangement of expanded and contracted NiO₆ octahedra, naturally explained by a three-sublattice charge order pattern on the triangular lattice of Ni sites. Band-structure calculations suggest that charge order occurs in order to lift the orbital degeneracy and is favoured by the weak electron delocalization over local Jahn Teller distortions found in more insulating systems. An unusual magnetic order is observed at low temperatures with only one third of sites (the electron-rich Ni sites) carrying a magnetic moment arranged in an unexpected collinear stripe order pattern on an antiferromagnetic triangular lattice. Possible mechanisms stabilizing the observed ground state will be discussed. E. Wawrzynska, R. Coldea, E. M. Wheeler, I. I. Mazin, M. D. Johannes, T. Sörgel, M. Jansen, R. M. Ibberson, P. G. Radaelli, Phys. Rev. Lett. 99, 157204 (2007). We acknowledge support from EPSRC UK.

2:54PM D23.00003 Neutron scattering investigation of Lithium based spinels. WOUTER MONT-FROOU. MARCUS PETROVIC, MICHAEL KRAUS, University of Missouri, ALEXANDER SCHMETS, Technical University Delft — Lithium based spinels LiₓM₂O₄, (with M a transition metal like Mn, V, Ti) offer a rich variety of ground states, depending on the transition metal in question. What makes these materials particularly attractive for both fundamental research as well as for applications is that the Li atoms can easily be extracted from the crystal without affecting the overall spinel structure. The oxidation state of the mixed valent transition metal M will change as a function of Li removal, with the result that the system can go from a disordered state to a long range ordered state. We present new neutron scattering results on a variety of Lithium spinels [LiₓMn₂O₄, LiCoO₂, LiCoₓFe₁₋ₓO₂, LiNiVO₄, and LiNiₓFeₓOₓVO₄]. We discuss the changes in ground states as a function of Lithium content, and we review how the magnetic properties of the transition metal ions influence the electronic properties of the system.

3:06PM D23.00004 Elastic properties of the vanadate spinel MnV₂O₄. V. KEPPENS, Y. LUAN, Dept. Materials Science and Engineering, The University of Tennessee, V.O. GARLEA, Neutron Scattering Sciences Division, Oak Ridge National Laboratory, R. JIN, D. MANDRUS, Materials Science and Technology Division, Oak Ridge National Laboratory — Spinel vanadates AV₂O₄ are known to undergo a cubic-to-tetragonal structural phase transition (SPT) at temperature Tₛ and order magnetically at lower temperature Tₓ. ZnV₂O₄ is characteristic of the entire series and has received extensive theoretical attention. When Mn occupies the A site there is an additional supereexchange interaction between Mn and V. This superechange interaction leads to ferrimagnetic order at about 56 K, involving a ferromagnetic configuration of the V spins. The current work focuses on the elastic properties of MnV₂O₄. Resonant Ultrasound Spectroscopy (RUS) has been used to measure the elastic response of the sample, as a function of temperature (5-300K) and magnetic field (0-7 Tesla). The temperature dependence of the frequencies is found to be quite unusual, displaying a softening over a large temperature range. Measurements in magnetic field reveal an additional feature near 50 K, which could represent a striking manifestation of direct spin-orbital coupling.

3:18PM D23.00005 Neutron Scattering Study of Magnetic and Orbital Order in MnV₂O₄. STEPHEN NAGLER, OVIDIU GARLEA, Oak Ridge National Laboratory, RONYING JIN, DAVID MANDRUS, DOUG ABERNATHY, Oak Ridge National Laboratory, BERTRAND ROESSLI, Paul Scherrer Institute, MARTHA MILLER, ARTHUR SCHULTZ, Paul Scherrer Institute, MARTHA MILLER, ARTHUR SCHULTZ, Argonne National Laboratory, QINGZHEN HUANG, NIST Center for Neutron Research, CHRIS FROST, Rutherford-Appleton Laboratories — Neutron diffraction and inelastic scattering has been used to study the spinel system MnV₂O₄. The results confirm the existence of two phase transitions. The first, near 56 K, is from a paramagnetic state to a collinear ferrimagnetic phase. There is a second simultaneous structural and magnetic transition at 53 K to a tetragonal structure with a non-collinear ferrimagnetic state. The low-T magnetic structure has been definitively resolved, and is seen to be associated with a gap in the magnetic excitation spectrum. The magnetic structure is compatible with a staggered orbital ordering. Inelastic scattering has been carried out using both triple axis and time of flight techniques, and several branches of magnetic excitations are visible. These observations put tight constraints on theoretical models for MnV₂O₄. An initial account of some of the results of this work appears in arXiv:0711.1844v1.

3:30PM D23.00006 Magnetic and magnetoelastic properties of Ge-substituted cobalt ferrite. NARESH RANVANH, IKENNA NLEBEDIM, Cardiff University, YEVGEN MELIKHOV, JOHN SNYDER, DAVID JILES, ANTHONY MOSES, PAUL WILLIAMS, Cardiff University, WOLFSON CENTRE FOR MAGNETICS TEAM — Research in past has shown chemical substitution of Fe²⁺ by trivalent ions (Cr³⁺, Mn³⁺ and Ga³⁺) to alter the properties of these materials, notably reducing Curie temperature and magnetic anisotropy, which lead to increase in permeability. The change in properties has been understood in terms of site preference of the dopant cation. Since its discovery, it has been studied as a minor structural impurity phase in CMR-related CaMnO₃. It was first described [1] in 1963 as a natural mineral called Marokite. Since its discovery, it has been studied as a minor structural impurity phase in CMR-related CaMnO₃ and for its structural similarities to high-pressure phases of spinel-oxide compounds. However, little attention has previously been paid to physical transport, thermal transport, thermal expansion, heat capacity, and magnetization.

CaMnO₃ was first described [1] in 1963 as a natural mineral called Marokite. Since its discovery, it has been studied as a minor structural impurity phase in CMR-related CaMnO₃. What makes these materials particularly attractive for both fundamental research as well as for applications is that the Li atoms can easily be extracted from the crystal without affecting the overall spinel structure. The oxidation state of the mixed valent transition metal M will change as a function of Li removal, with the result that the system can go from a disordered state to a long range ordered state. We present new neutron scattering results on a variety of Lithium spinels [LiₓMn₂O₄, LiCoO₂, LiCoₓFe₁₋ₓO₂, LiNiVO₄, and LiNiₓFeₓOₓVO₄]. We discuss the changes in ground states as a function of Lithium content, and we review how the magnetic properties of the transition metal ions influence the electronic properties of the system.

4:18PM D23.00008 Electrical, Thermal, and Magnetic Properties of Single Crystal CaMn₂O₄ Marokite. B.D. WHITE, J.J. NEUMEIER, J.A. SOUZA, Montana State University, C. CHIORESCU, J.L. COHN, University of Miami — CaMnO₃ was first described [1] in 1963 as a natural mineral called Marokite. Since its discovery, it has been studied as a minor structural impurity phase in CMR-related CaMnO₃ and for its structural similarities to high-pressure phases of spinel-oxide compounds. However, little attention has previously been paid to physical properties beyond its temperature-dependent magnetization. We will present a detailed physical properties study of CaMn₂O₄ single crystals grown by the optical floating zone method. [2] These measurements, several of which display anisotropy as a result of an orthorhombic crystal structure, include electrical transport, thermal transport, thermal expansion, heat capacity, and magnetization.


This material is based upon work supported by the NSF (Grant No. DMR-0504769 at MSU and DMR-0072276 at U. Miami), the Research Corporation and the U.S. DOE Office of Basic Energy Sciences (Grant No. DE-FG-06ER46269).
4:30PM D23.00009 X-ray diffraction and reciprocal space mapping in ZnMnGaO$_4$ films with checkerboard nanostructures, A.A. SIRENKO, S.M. O’MALLEY, P.L. BONANNO, Department of Physics, New Jersey Institute of Technology, Newark, New Jersey 07102, A. KAZIMIROV, Cornell High Energy Synchrotron Source (CHESS), Cornell University, Ithaca, New York 14853, S. PARK, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854 — Reciprocal space maps (RSM) in ZnMnGaO$_4$ films with checkerboard nanostructures were measured with the energy of the x-ray beam of 10.53 keV at the A2 beamline at Cornell High Energy Synchrotron Source (CHESS) using a four-circle diffractometer. Structural properties of the checkerboards, such as elastic strain, relaxation effects, twists, and tilts of the nanodomains, were analyzed using H-K, H-L, and K-L cross sections of the RSM’s measured around various symmetric and asymmetric reflections (022), (004), (044), (226), (222) of the spinel structure. Work at Rutgers was supported by the DE-FG02-07ER46382 and the NSF-DMR-0706326. Work at NJIT was supported by the NSF-DMR-0540985. The Cornell High Energy Synchrotron Source is supported by the NSF and the NIH/NIGMS under Award No. DMR-0225180.

4:42PM D23.00010 Magnetic coupling in CoCr$_2$O$_4$ and MnCr$_2$O$_4$; an LSDA+U study, CLAUDE EDERER, Trinity College Dublin, Ireland, MATEJ KOMELJ, Jožef Stefan Institute, Ljubljana, Slovenia — Competing magnetic interactions can lead to very interesting magnetic structures and pronounced effects due to spin-lattice coupling. Chromium spins with additional magnetic $A$-site cations are prime examples for such systems, and have recently regained attention due to the discovery of a small electric polarization in CoCr$_2$O$_4$ [1]. The multiferroic character of CoCr$_2$O$_4$ is supposedly a result of its inversion symmetry-breaking magnetic structure, which has been classified as a “ferromagnetic spiral” [2]. To achieve a better understanding of the complicated magnetic structure in CoCr$_2$O$_4$ and similar systems, an ab initio determination of the magnetic coupling constants is very desirable. Here, we present results of LSDA+U calculations of the magnetic coupling constants in both CoCr$_2$O$_4$ and MnCr$_2$O$_4$ [3]. We carefully assess the predictive power of such calculations, and then give quantitative estimates for the strengths of the most prominent magnetic interactions. Our results highlight the possible importance of $A$ interactions in spin systems with magnetic ions on both $A$ and $B$ sites, and provide an important link between previous theory and experimental observations.


4:54PM D23.00011 Crystal and Magnetic Structure of FeV$_2$O$_4$ with $e_g$ and $t_{2g}$ orbital degeneracies, SUNGDAE JI, J.-H. KIM, S.-H. LEE, Department of Physics, University of Virginia, Charlottesville, VA 22904, USA, Q. HUANG, NIST Center for Neutron Research, Gaithersburg, MD 20899, USA, T. KATSUFUJI, Department of Physics, Waseda University, Tokyo 169-8555, Japan — We have performed neutron diffraction measurements on a powder and a single crystal of a spinel FeV$_2$O$_4$ that has $e_g$ as well as $t_{2g}$ orbital degeneracy. Our data show that upon cooling this system undergoes three successive phase transitions: a cubic-to-tetragonal structural transition at 140 K, a tetragonal-to-orthorhombic transition at 110 K accompanied by a ferri-magnetic order and an orthorhombic-to-orthorhombic phase transition with another magnetic order at 80 K. The magnetic structures of the two magnetic phases were refined by the group theoretical analysis of our powder diffraction data. We will also discuss implication of the magnetic structures regarding to the orbital states of FeV$_2$O$_4$.

5:06PM D23.00012 ABSTRACT WITHDRAWN —

5:18PM D23.00013 The Dzyaloshinskii-Moriya Anisotropy in Hyper-Kagome Lattice for Na$_3$Ir$_4$O$_8$, GANG CHEN, LEON BALENTS, UCSB — The effect of quantum correction on the classical spin order in the iridium antiferromagnet Na$_3$Ir$_4$O$_8$ are considered. The spin-wave spectrum is calculated to the linear order. The nearest-neighbor exchange interactions between the Irspins as well as the Dzyaloshinskii-Moriya interactions are taken into account. Numerical simulation by exact diagonalization and experimental results are used to compare with the theoretical prediction.

Monday, March 10, 2008 2:30PM - 4:42PM — Session D24 DCMP: Superlattices and Nanostructures: Electronic Properties I

2:30PM D24.00001 Recent Progress on Modeling H Passivated CdS Nanocrystals using ab initio techniques, CHAD JUNKERMEIER, JINLING ZHOU, JAMES P. LEWIS, Dept. of Physics, West Virginia University — Spherical CdS nanocrystals with shells of H atoms are studied via an ab initio tight-binding analysis. Starting from the bulk zinc blende structure of CdS, these nanocrystals undergo relaxation as the geometries optimize to configurations that minimize internal forces. H atoms are then attached, to passivate the surface, and then whole structure is relaxed. We will present our latest results.

3This research is funded in part by the National Institute of Standards and Technology grant number 70NANB7H6008. This work was supported in part by a grant from the West Virginia Graduate Student Fellowships in Science, Technology, Engineering and Math.

4Also at: Dept. of Physics and Astro., Brigham Young University

2:42PM D24.00002 Measurements of Charge Transport in Arrays of Lead Selenide Nanocrystals, KENNETH MACLEAN, TAMAR MENTZEL, SCOTT GEYER, VENDA PORTER, MOUNGI BAWENDI, MARC KASTNER, Massachusetts Institute of Technology — We report electrical transport measurements of self-assembled arrays of PbSe nanocrystals (NC). NCs ~6.2 nm in diameter are colloidally synthesized and drop cast onto an inverted field effect structure. The NCs self assemble into hexagonal close-packed arrays with ~2 nm interparticle spacing. The current is immeasurable in as deposited arrays. After annealing at 400K for ~30 minutes, the arrays become less ordered and the conductance increases by more than 6 orders of magnitude. We measure the current in these devices as a function of source-drain voltage, gate voltage and temperature. We find that the temperature dependence of the conductance is strong at zero-bias and grows weaker with application of a source-drain bias. This implies that the conductance is thermally activated and the field serves to reduce the activation energy. We also find that the gate modulates the activation energy to conduction.

1We acknowledge support from NSF MRSEC (DMR-0213282), NSF NSEC (DMR-0117795), US Army Research Office (DAAD 19-02-0002)
2:54PM D24.00003 Structural and Electronic Properties of IV-VI Semiconductor Nanodots, ROMAN LEITSMANN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena — The characterization of nanostructure properties versus dimension and surface passivation is of increasing importance for the nanotechnology. Especially the stoichiometry, geometry, and the electronic states of IV-VI semiconductor nanodots are of special interest [1, 2]. We use ab initio methods to calculate structural and electronic properties of colloidal IV-VI semiconductor nanodots as a function of the dot diameter. A method to passivate the non-directional dangling bonds at the nanodot surfaces is derived and used to study the confinement effect on the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) states. In addition we take the influence of relativistic (spin-orbit coupling – SOC) and excitonic effects into account. While the SOC leads to a considerable decrease of the HOMO-LUMO gap, excitonic effects play a minor role. [1] JACS 128, 10337 (2006) [2] JACS 129, 11354 (2007)

3:06PM D24.00004 Density functional theory studies of core-shell semiconductor nanoparticle quantum dots, BRENT WALKER, SHAUN HENDY, Industrial Research Limited, 69 Gracefield Road, P.O. Box 31-310, Lower Hutt 5040, New Zealand, RICHARD TILLEY, School of Chemical and Physical Sciences, Victoria University of Wellington, P. O. Box 600, Wellington, New Zealand — In going from the macroscale to the nanoscale, quantum-mechanical effects become increasingly important and may mean that nanostructures of a material exhibit very different properties from the corresponding bulk. This is especially noticeable in the case of the optical properties of semiconductor nanoparticles (or quantum dots), which display a number of remarkable features (including very distinct peaks, and tunability across a broad range of wavelengths), due to quantum confinement. Our work involves modeling Si-Ge core-shell nanoparticles using large-scale computer simulations based on the density functional and time-dependent density functional theories. These simulations in particular provide us with predictions of the geometric structures and optical absorption spectra of nanoparticles in an accurate and computationally efficient way, and allow us to study the systematic trends in these properties as the composition and size of the nanoparticle change.

3:18PM D24.00005 Conduction Mechanism in Arrays of Lead Selenide Nanocrystals, TAMAR MENTZEL, KENNETH MACLEAN, SCOTT GEYER, VENDA PORTER, MOUNGI BAWENDI, MARC KASTNER, Massachusetts Institute of Technology — We perform transport measurements of a PbSe nanocrystal solid which serves as the channel of a field-effect transistor. We find that a simple model of hopping between intrinsic localized states describes the conduction mechanism. From the field effect, we see that the majority carriers are holes, which are thermally released from acceptor states. At low source-drain voltages, the activation energy for the conductivity is given by the energy required to generate holes plus the activation over barriers resulting from site disorder. At high source-drain voltages the activation energy is given by the former only. The thermal activation energy of the zero-bias conductance indicates that the Fermi energy is close to the highest-occupied valence level, the 1S, state, and this is confirmed by field-effect measurements, which give a density of states of approximately 8 per nanocrystal as expected from the degeneracy of the 1S, state. Using the Thomas-Fermi screening length in the NC solid, we find that the gate serves to modulate the charge density in the monolayer closest to the gate, while successive monolayers are screened from the field.

3:30PM D24.00006 Quasi 1-D electronic structure of silver nanowires, A. SEKHARAN, W. ZHAO, F. WOMACK, F. WANG, O. KIZILKAYA, R. KURTZ, P. SPRUNGER, Louisiana State University — Epitaxial Ag nanowires have been found to self-assemble on Cu(110) at coverages exceeding 1.2 ML. The low energy electronic structure of these nanowires has been characterized by ARPES. Previous STM, LEED, and LEEM data reveal that the Ag nanowires grown on Cu(110) are approximately 2 nm (∼12 nm) in height (width). The nanowires orient with the long axis parallel to the [1 1 0] substrate direction. The ARPES results reveal that the valence bands within the Ag nanowire are strongly anisotropic with clear band dispersion in the along-wire direction, but no dispersion in the across-wire direction. ARPES identified two low-energy electronic bands, with strong dispersion close to the Fermi energy. The first band, which crosses the Fermi energy, suggests the metallic nature of nanowires. However, there is an avoided crossing of the second band, perhaps due to many-body effects. While discussing the quasi 1-D electronic structure, we will emphasize its connection to many-body effects and the one dimensional nature of nanowires.

3:42PM D24.00007 ABSTRACT WITHDRAWN —

3:54PM D24.00008 Measurements of the conduction band energy surrounding individual InGaAs quantum dots by Cross-Sectional Ballistic Electron Emission Microscopy (XBEEM), C. MARGINEAN, J.P. PEIZ, The Ohio State University, S.Y. LEHMAN, The College of Wooster, J.G. CEDERBERG, Sandia National Laboratories — Cross-sectional ballistic electron emission microscopy (XBEEM) at room temperature was used to measure the conduction band (CB) energy in the “wetting layer” around and behind cleaved InGaAs quantum dots (QDs). Samples with a ∼2 nm thick In0.4Ga0.6As layer embedded in n-doped (5 × 1013 cm−3) GaAs were grown by organometallic vapor phase epitaxy, then cleaved ex situ, and 7nm-thick Au Schottky barrier (SB) contacts deposited on the cleaved edge using a shadow mask [1]. With reverse bias Vrev = 0V, Schottky barrier heights (SBHs) over different QDs were measured to range from ∼0.78 eV − 0.82 eV, compared to ∼ 0.84 eV over the wetting layer next to the QDs and ∼0.913 eV SBH over the adjacent GaAs. With Vrev = 1V, the SBH over the QDs were reduced by ∼30 – 50 meV compared to a much smaller (< 5 meV) measured decrease over the GaAs due to image force lowering, indicating that SBH over the QDs was due to the CB of the wetting layer at an estimated depth of 6 – 9 nm behind the QDs. The XBEEM transmission over the QDs was also strongly enhanced by the applied reverse bias, for reasons that are not yet clear. Work supported by NSF Grant No. DMR-0505165. [1] C. Tivaros et al., PRL 94, 206803 (2005).

4:06PM D24.00009 Shifting the Reference: Co on Cu(775), M.B. YILMAZ, S. WANG, K.R. KNOX, N. ZAKI, J.I. DADAP, R.M. OSGOOD, Brookhaven National Laboratory — The conduction band energy of a semiconductor substrate can be shifted with respect to an energy reference frame. We report on the use of a metal Schottky contact to shift the reference frame to a 1-nm-thick Cu film and measure the conduction band energy (Ecb) of nanostructured Co/Cu(775). The measured Ecb of the Cu film was 0.6 eV, and of the Co/Cu(775) interface was 0.2 eV. Work supported by DOE Contract Nos DE-FG02-04ER46157 and DE-AC02-98CH10886.

1Supported in part by NSF/DMR-0504654 and LA-R&D.

2Supported by NSF MRSEC, NSF NSEC, US ARO. TM acknowledges support from NSF GRFP.
4:18PM D24.00010 Experimental separation of entanglements in polymer blends. ERICA SALTZMAN, MURUGAPPAN MUTHUKUMAR, University of Massachusetts at Amherst — We have developed a quantum holographic method to advance information density beyond the areal limits set by the discreteness of matter. We present experiments on information encoding using nonscale writing with degenerate two-dimensional electrons. We show "pages" (letters encoded at specific energies) materialized by precisely engineering electron scattering environments with the tip of a scanning tunneling microscope. We then demonstrate that multiple pages can be encoded into the same region of space, using energy as a third holographic dimension.

This form of holography produces non-volatile subnanometer features, tens of times smaller than the most precise optical or scanned-probe lithography, and information densities exceeding 5 bits per square nanometer.

1Supported by ONR, NSF, and DOE.

4:30PM D24.00011 Exploiting Resonances in Laser Photoemission1 . J.J. DADAP, M.B. YILMAZ, K. KNOX, N. ZAKI, R.M. OSGOOD, Columbia University. P.D. JOHNSON, Brookhaven National Laboratory — Laser photoemission is attracting new interest due to its ability to increase photoemission probe depth and to gain insight into surface-electron dynamics. We present new data on the use of energy levels that are resonant with the excitation-photon energy. Our surface system is the regular array of nanometer-scale steps on Cu(775), which yield information on surface electron confinement. We probe this nanostructured system with 2-photon photoemission. Our tunable, fs optical parametric amplifier (OPA) source allows resonance mapping with photon energies ~ 4.2-4.6 eV to obtain a comprehensive map of the unoccupied state manifold. We observe, in addition to the surface state and image states, bandfolding from Umklapp due to the periodic steps, and, for the first time, the existence of a weak unoccupied state. The OPA allows observation of even this relatively weak unoccupied state as well as the rapid interrogation of electronic structure. The origin of this intermediate state is discussed. In addition, we present the intensity dependence of the measured linewidth and the position of the resonances.

1This work is supported by DOE contracts DE-FG02-04ER46157 and DE-AC02-98CH10886.

Monday, March 10, 2008 2:30PM - 5:30PM — Session D25 DPOLY: Theory and Simulations I Morial Convention Center 217

2:30PM D25.00001 Thermodynamically Consistent Nonrandom Mixing on a Bethe Lattice . SCOTT MILNER, ExxonMobil — For over 40 years, engineering calculations of nonrandom mixing effects in lattice-based calculations of free energies of mixing in both small-molecule and polymeric solutions (e.g., the non-random two-liquid model, or NRTL) have been based on a strange approximation. By "strange", I mean that the approximation violates some commonsense sum rules in how the lattice is filled; namely, that "something is next to everything"; and "everything is next to something". The resulting theories are thermodynamically inconsistent, and explicitly depend on combinations of interaction energies of which the exact mixing free energy is demonstrably independent. To remedy this, I have extended the exact solution of the Ising model on a Bethe lattice to an n-component mixture with arbitrary pairwise interactions. Explicit and practical expressions are obtained for the entropy and average energy per site, which incorporate nonrandom mixing in a thermodynamically consistent way. Although it still has mean-field exponents for the binary mixture critical point, the shape of the coexistence curve lies much closer to the exact results for the Ising model in d = 3 dimensions than do previous engineering-level theories. In addition, the model may be generalized easily to deal with mixtures of species occupying different numbers of sites on the lattice. Thus the model can be used to compute phase behavior for mixtures of molecules of different sizes, including polymeric solutions.

2:42PM D25.00002 Mixture Properties of Flexible Chains: Comparisons between Experiment, Simulation and Theory; Contrasts between Lattice and Continuum . RONALD WHITE, JANE LIPSON, Dartmouth College — We present new theoretical results for a series of binary chain-molecule mixtures using both the hard-sphere, and the square-well potentials. We compare these results to simulation data, and contrast them to those obtained using the analogous lattice version of the theory. We discuss all of our findings in the context of experimental data for hydrocarbon chain mixtures. In the course of these studies we consider mixtures of components with varied chain lengths and energetics, and examine the effects of changing composition, temperature, and density. In addition, by calculating the free energy over a wide range of the P,V,T and composition space, we are able to characterize coexistence, both liquid-vapor as well as liquid-liquid partial miscibility.

2:54PM D25.00003 A Multichain Self-Consistent Field Theory for Correlations in Polymers: Chain Swelling in Polymer Blends . DAVID WU, Colorado School of Mines — The self-consistent mean field theory of polymers has been highly successful as a tractable computational framework for capturing the thermodynamics and structure of polymer systems. One notable limitation has been the neglect of fluctuations and correlations, which can be important in a variety of physical circumstances. One such circumstance involves the non-Gaussian conformations (swelling) of branched polymers. We present a method for calculating these correlations with an extension of the SCF theory when applied to multiple chains. As an example of the methodology, we show how the crossover from swollen to screened conformations occurs in a blends of star and linear polymers.

3:06PM D25.00004 Numerical Renormalization Group for Coarse Graining Field-Theoretic Fluid Models . MICHAEL VILLET, GLENN FREDRICKSON, University of California, Santa Barbara — Statistical field theory models have proven to be valuable tools for studying the equilibrium behavior of polymeric fluids, but direct simulation of these field theories without use of the mean field approximation is computationally demanding. Computational resources can be extended to simulate larger systems by discretizing the field variables with a coarsely spaced lattice, but indelicate coarse graining risks truncation of important short-wavelength physics. We investigate numerical renormalization group transformations in tandem with complex Langevin simulations as a systematic approach to coarse graining field-theoretic fluid models, using a simple repulsive Yukawa fluid as a test system.

3:18PM D25.00005 Continuous translocations in connected chambers under pseudo-hydrodynamic force . ERICA SALTZMAN, MURUGAPPAN MUTHUKUMAR, University of Massachusetts at Amherst — Experimental separation of polydisperse synthetic and biopolymers is frequently conducted via combination of electrophoretic or hydrodynamic flow with a series of obstacles or traps. In order to understand the interaction of entropic escape and biased diffusion processes, we conduct simulations on a generic model system. Brownian dynamics simulations are performed on linear chains confined in a series of chambers connected by narrow pores. A uniaxial force designed to mimic the effect of solvent flow acts on each bead of the chain, leading to translocation between chambers. Translocation events are separated by periods of trapping, which shorten with increasing chain length; for long chains individual translocations become indistinguishable.
A two-scale-two-mode dynamic self-consistent theory of entangled interfaces in polymer fluids under flow. YITZHAK SHNIDMAN, ISMAEL YACOUBOU-DJIMA, College of Staten Island. City University of New York — Tracking conformation statistics on the Kuhn scale is essential for modeling interfacial phenomena in polymer fluids under flow. Successive entanglements partition entangled chains into strands that are in one of two modes: entangled or dangling. Strands follow different differential evolution equations for the second moment of their end-to-end distance, depending on their mode. Dangling strands are governed by the FENE-P equation. For entangled strands, a different evolution equation was proposed by G. Marrucci and G. Ianniruberto, Phil. Trans. R. Soc. Lond. A 361, 677 (2003). On the Kuhn scale, strand’s conformation statistics is sampled by random walks in an effective potential, which are regulated by the evolving second moment of its end-to-end distance. Conformation statistics of a dangling strand is adequately modeled by Wiener (uncorrelated) random walks, but stretching of entangled strands under flow induce correlations between successive steps requiring a persistent random walk model (I. Yacoubo-Djima and Y. Shnidman, http://arxiv.org/abs/0708.2679v1). A two-scale-two-mode subchain propagation scheme, starting from free segments evolved by a probabilistic transport equation, allows a self-consistent calculation of evolving interfacial structure and rheology.

A new approach to the glass transition temperature $T_g$ in polymer fluids under flow. Successive entanglements partition entangled chains into strands that are in one of two modes: entangled or dangling. Strands follow different differential evolution equations for the second moment of their end-to-end distance. Dangling strands are governed by the FENE-P equation. For entangled strands, a different evolution equation was proposed by G. Marrucci and G. Ianniruberto, Phil. Trans. R. Soc. Lond. A 361, 677 (2003). On the Kuhn scale, strand’s conformation statistics is sampled by random walks in an effective potential, which are regulated by the evolving second moment of its end-to-end distance. Conformation statistics of a dangling strand is adequately modeled by Wiener (uncorrelated) random walks, but stretching of entangled strands under flow induce correlations between successive steps requiring a persistent random walk model (I. Yacoubo-Djima and Y. Shnidman, http://arxiv.org/abs/0708.2679v1). A two-scale-two-mode subchain propagation scheme, starting from free segments evolved by a probabilistic transport equation, allows a self-consistent calculation of evolving interfacial structure and rheology.

Fluctuations in Confined Homopolymers Studied by Fast Off-Lattice Monte Carlo Simulations. YUHUA YIN, QIANG WANG — The conventional molecular simulations of many-chain systems are hindered by explicit excluded-volume interactions and expensive pair-potential calculations. The former greatly reduces the chain relaxation towards equilibrium configurations and the efficiency of sampling the configurational space, while the latter becomes computationally very expensive for concentrated polymeric systems. Fast off-lattice Monte Carlo (FOMC) simulations overcome these limitations, where individual polymer segments are modeled as volumeless points with the excluded-volume interactions modeled by either solvent quality, Helfand compressibility, or incompressibility constraint commonly used in polymer field theories. By dividing the simulation box into cells and assigning polymer segments to a cell, the short-range interactions can be readily evaluated without expensive pair-potential calculations. To demonstrate the great advantages of FOMC simulations, we have studied homopolymers confined between two parallel surfaces, and compared the results with self-consistent field calculations and field-theoretic simulations (FTS). Since FOMC simulation is particle-based, it avoids the unsolved 7sign problem encountered in FTS. For the systems we have studied, FOMC simulations can sample the whole spectrum of fluctuations and are several orders of magnitude faster (more efficient) than FTS.
Para = 2 – 100 %

cryogenic nozzle beam expansion of a neat

doped in H

of bulk H

correlations and scattering structure factors as phase separation is approached has been studied in detail.

mean force can occur, which raises the possibility that kinetic gelation or aggregation pre-empts equilibrium phase separation. The evolution of the real space

by a highly asymmetric spinodal boundary which depends sensitively on attraction spatial range. Deep contact or bridging minima in the particle potential of

present, separated by a miscibility window. Entropic effects dominate for weak interfacial attractions (high temperature) resulting in depletion phase separation

boundaries compared to a low order virial treatment. In the temperature-particle volume fraction representation both upper and lower critical temperatures are

investigate phase separation and structure of dense mixtures of hard spherical particles and flexible polymer chains in the presence of interfacial attractive

interactions. The entire range of filler loading, from the dilute particle regime to the colloid science relevant case of ultra-high particle volume fraction with
dilute polymer additives, has been studied for the first time. Many body effects can result in large quantitative, or even qualitative, changes of spinodal demixing

boundaries compared to a low order virial treatment. In the temperature-particle volume fraction representation both upper and lower critical temperatures are

present, separated by a miscibility window. Entropic effects dominate for weak interfacial attractions (high temperature) resulting in depletion phase separation

with a critical point at roughly 10% filler loading. At relatively high interfacial cohesion (low temperature) a network bridging transition occurs characterized by a highly asymmetric spinodal boundary which depends sensitively on attraction spatial range. Deep contact or bridging minima in the particle potential of

mean force can occur, which raises the possibility that kinetic gelation or aggregation pre-empts equilibrium phase separation. We use this approach to study the role


5:06PM D25.00014 Conformation and collapse of a polymer chain in explicit solvent: A solvation potential approach , MARK P. TAYLOR, Dept. of Physics, Hiram College, Hiram, OH — The conformation of a polymer chain in solution is intrinsically coupled to the chain’s local solvent environment. In much of the theoretical work on polymers in solution the effects of solvent are treated implicitly and explicit chain-solvent coupling is ignored. Although a formally exact treatment of chain-solvent coupling can be constructed, the required many-body solvation potential is not practical to compute. We have recently shown that for short hard-sphere and square-well chain-in-solvent systems this many-body solvation potential can be made tractable via an “exact” decomposition into a set of two-site potentials [1]. Here we use these exact short chain results, combined with the pure solvent potential of mean force, to construct approximate two-site solvation potentials for long chains under a range of solvent conditions [2]. Monte Carlo simulations for full chain-in-solvent systems verify the accuracy of our solvation potential approach. We use this approach to study the role of driving and inhibiting chain collapse in square-well systems and discuss the possibility of solvent driven chain collapse in the symmetric hard-sphere chain-in-solvent system. [1] M. P. Taylor and G. M. Petersen, J. Chem. Phys. 127, 184901 (2007). [2] M. P. Taylor and S. Ichida, J. Polym. Sci., Part B: Polym. Phys. 45, 3319 (2007).

5:18PM D25.00015 Statistical Mechanical Theory of Phase Separation and Structure in Dense Polymer-Particle Mixtures , LISA HALL, KEN SCHWEIZER, University of Illinois — Microscopic liquid state theory has been applied to investigate phase separation and structure of dense mixtures of hard spherical particles and flexible polymer chains in the presence of interfacial attractive interactions. The entire range of filler loading, from the dilute particle regime to the colloid science relevant case of ultra-high particle volume fraction with dilute polymer additives, has been studied for the first time. Many body effects can result in large quantitative, or even qualitative, changes of spinodal demixing boundaries compared to a low order virial treatment. In the temperature-particle volume fraction representation both upper and lower critical temperatures are present, separated by a miscibility window. Entropic effects dominate for weak interfacial attractions (high temperature) resulting in depletion phase separation with a critical point at roughly 10% filler loading. At relatively high interfacial cohesion (low temperature) a network bridging transition occurs characterized by a highly asymmetric spinodal boundary which depends sensitively on attraction spatial range. Deep contact or bridging minima in the particle potential of mean force can occur, which raises the possibility that kinetic gelation or aggregation pre-empts equilibrium phase separation. The evolution of the real space correlations and scattering structure factors as phase separation is approached has been studied in detail.

Monday, March 10, 2008 2:30PM - 5:30PM —
Session D26 DCP: Focus Session: Photophysics of Cold Molecules III Morial Convention Center 218

2:30PM D26.00001 Spectroscopy of large hydrogen clusters in He droplets and H2 droplets Ur, TAKAMASA MOMOSE, The University of British Columbia — Clusters of molecular hydrogen (H2) at low temperatures have been attracted much attention because of the possible superfluid phase of molecular hydrogen. Parahydrogen has been predicted to undergo Bose-Einstein condensate (BEC) and to exhibit a superfluid phase below 6 K. However, since the freezing point of H2 (14 K) is much higher than the predicted superfluid transition temperature, the supercooling of bulk H2 system has not been achieved despite many attempts. Clusters are known to exhibit lower freezing and melting temperatures than their bulk system due to the size effect. In addition, the melting temperature may become significantly lower than the freezing temperature in such clusters, and coexistence of liquid and solid phases between the melting and freezing temperatures has been predicted theoretically. Thus, clusters of molecular hydrogen are very appealing system for the observation of possible superfluid phase of molecular hydrogen. Since superfluid is a macroscopic property, we have studied properties of hydrogen clusters with fairly large size (N = 100 – 103) by using He droplet spectroscopy. Some advantages of using droplet spectroscopy for this study include (1) cluster size can be precisely controlled by its pickup process, and (2) the temperature of clusters is well defined. Laser induced fluorescence of several molecules doped in H2 clusters showed clear evidence of non-rigidity of hydrogen clusters at 0.4 K or 4 K. We have also observed a clear difference in the LIF spectra between parahydrogen and orthohydrogen clusters. We will discuss the properties of large parahydrogen clusters from the dependence on the cluster size and concentration of orthohydrogen.

3:06PM D26.00002 Hydrogen clusters that remained fluid Ur, KIRILL KUYANOV-PROZUMENT, ANDREY VILESOV — Para-H2 may constitute the only other superfluid besides helium. The superfluid transition temperature is predicted to be around 2 K, well below freezing of H2 at 13.8 K. Numerous attempts to supercool macroscopic H2 samples proved to be unsuccessful. Our approach includes formation of H2 clusters in a pulsed cryogenic nozzle beam expansion of a neat p=H2 gas as well as x% of p=H2 diluted in He and interrogation via Coherent Anti-Stokes Raman Scattering. At X = 2 – 100 % the frequency of the vibrational Q1(0) line in clusters remains constant at v = 4149.7 cm−1 very similar to 4149.6 cm−1 as in solid p=H2 and lower than in liquid p=H2at 18 K (4151.9 cm−1). The rotational S0(0) transition show some characteristic crystal field splitting having magnitude of about 6 cm−1. The splitting pattern is different from that in the hcp solid, suggesting different structure in solid p=H2 clusters. At X < 2 %, the frequency of the Q1(0) line increases to about 4150.5 cm−1, which is consistent with that expected in the supercooled liquid. The S0(0) transition in these clusters, consisting of about 5 x 104 molecules, appears as a single line at the same frequency as in liquid p=H2. The temperature of these supercooled clusters is estimated to be less than about 1 K. Possible superfluidity of the clusters is discussed.

3:18PM D26.00003 Three-body interactions in liquid and solid hydrogen: Evidence from vibrational spectroscopy , ROBERT HINDE, Univ. of Tennessee — In the cryogenic low-density liquid and solid phases of H2 and D2, the H2 and D2 molecules retain good rotational and vibrational quantum numbers that characterize their internal degrees of freedom. High-resolution infrared and Raman spectroscopic experiments provide extremely sensitive probes of these degrees of freedom. We present here fully-first-principles calculations of the infrared and Raman spectra of liquid and solid H2 and D2, calculations that employ a high-quality six-dimensional coupled-cluster H2–H2 potential energy surface and quantum Monte Carlo treatments of the single-molecule translational degrees of freedom. The computed spectra agree very well with experimental results once we include three-body interactions among the molecules, interactions which we also compute using coupled-cluster quantum chemical methods. We predict the vibrational spectra of liquid and solid H2 at several temperatures and densities to provide a framework for interpreting recent experiments designed to search for superfluid behavior in small H2 droplets. We also present preliminary calculations of the spectra of mixed H2/D2 solids that show how positional disorder affects the spectral line shapes in these systems.
3:30PM D26.00004 Rotational spectrum of small, doped 3He clusters . TATJANA SKRBIĆ, SISSA - DEMOCRITOS (Trieste, Italy), SAVERIO MORONI, DEMOCRITOS - SISSA (Trieste, Italy), STEFANO BARONI, SISSA - DEMOCRITOS (SISSA) — In recent years, symmetry-adapted imaginary-time correlation functions have been extensively used to study the rotational spectrum of doped 3He clusters within the frame of the repulsion quantum Monte Carlo method. The success of this approach relies on the choice of suitable correlation functions, whose spectral resolution is dominated by few, well separated eigenvalues of the Hamiltonian. Under these conditions, reliable excitation energies can be extracted by inverse Laplace transform. This method has been tailored for bosons, due to the positivity of the ground-state wave-function and to the distinctive scarcity of low-lying states. For sufficiently small systems, however, the states of the discrete spectrum can be calculated in the same manner also with Fermi statistics, using appropriate generalizations of the correlation functions. We present rotational spectra for small 3He clusters doped with molecules –such as CO2 and OCS– whose effective moments of inertia, in 4He clusters, feature a non-trivial dependence on the system size, with a pronounced turnaround for less than 10 atoms.

3:42PM D26.00005 Quantum melting and superfluidity of molecular hydrogen clusters , MASSIMO BONINSENGI, University of Alberta — Clusters of parahydrogen comprising between 10 and 50 molecules have been extensively studied by computer simulations based on the continuous-space Worm Algorithm, which allows one to go down to temperatures as low as a few hundredths of a K. These clusters display an intriguing interplay of liquid- and solid-like behavior as a function of both temperature and cluster size. In this sense, their physics is far richer than that of helium clusters. An intriguing phenomenon predicted by our simulations is quantum melting, whereby clusters in some size range (roughly between 22 and 30 molecules) are observed to go from rigid, solid-like, to essentially structureless and liquid-like as the temperature is lowered, due to the onset of quantum exchange cycles involving all the molecules in the cluster. At low temperature these clusters turn superfluid; their local superfluid response has been analyzed, and found to be essentially uniform throughout the system in the $T \to 0$ limit, even in clusters with a pronounced shell structure. In particular, exchanges involving molecules in the inner and outer shells are shown to be underlying the superfluid response. This system can also allow one to gain insight into the relationship of the superfluid properties with Bose condensation, and aspect that has been thoroughly investigated.

4:18PM D26.00006 Alkaline Earth Metal Atom Complexes with HCN Trapped On/In Helium Droplets: Vibrational Excitation Induced Solvation and Desolvation , GARY DOUBERY, University of Georgia — Infrared laser spectroscopy is used to probe the rotational dynamics of the binary HCN-M (M=Ca, Sr) complexes, either solvated within or bound to helium droplets. The “surface bound” spectral signatures reported previously for the HCN-alkali atom complexes are observed for both species, while a second band is observed for HCN-Ca that corresponds to a solvated species. IR-IR double resonance spectroscopy is used to probe the interconversion of the two distinct HCN-Ca populations. Above a threshold droplet size, vibrational excitation results in the solvation of the surface bound HCN-Sr complex.

4:30PM D26.00007 Imaging Photoelectron Dynamics in Doped Helium Droplets , CHIA WANG, University of California, Berkeley, OLEG KORNILOV, Lawrence Berkeley Nat’l Lab, DARCY PETERKA, JEONG KIM, OLIVER GESSNER, Lawrence Berkeley Nat’l Lab, DANIEL NEUMARK, University of California, Berkeley — Photoionization of He droplets doped with Xe and Kr atoms have been investigated by photoelectron imaging utilizing VUV synchrotron radiation. Photoelectron images were recorded over a wide range of He droplet sizes, photon energies, and dopant pick-up conditions. Significant ionization of dopants was observed at 21.6 eV, the absorption maximum of 2P electronic excited state of He droplets, suggesting an indirect ionization via excitation transfer. Photoelectron images and spectra indicate multiple pathways for photoelectrons generated by this process to escape the droplet. Special attention is paid to the excitation transfer dynamics and the electron relaxation in He droplets. It is found that excitation transfer from 2P state to dopants competes with relaxation to the lower 2S state. The excitation is likely a localized excitation that transfers the energy to the dopant via a dipole-dipole hopping mechanism. The conduction band of He droplets as a function of droplet size is also observed. The conduction band edge reaches the bulk limit for the largest He droplets. The electron under the conduction band becomes trapped and forms an electron bubble that escapes the droplet by transoncending a barrier near the liquid/vapor interface.

4:42PM D26.00008 Interchange-Tunneling Splitting in HCl Dimer in Helium Nanodroplets , DMITRY SKVORTSOV, RUSSELL SLITER, Univ of Southern California, MYONG YONG CHOI1, Gyeongsang National University, ANDREY F. VILESOV, Univ of Southern California — Infrared spectra of HCl dimers have been obtained in helium nanodroplets. The splitting in the vibrationally excited state of the bound HCl dimer (2ν) in (HCl - H2) dimers was observed to be 2.7 cm$^{-1}$ as compared to 3.7 cm$^{-1}$ in free dimer. From the splitting, the strength of the interchange-tunneling interaction in liquid helium was obtained to be 0.85 cm$^{-1}$, which is about a factor of two smaller than in the free dimer. The results are compared with the previous spectroscopic study of (HF)$_2$ in He droplets as well as to the theoretical study of (HF)$_2$ and (HCl)$_2$ dimers in small He clusters.

1Gyeongsang National University, Jinju, 660-701, South Korea

4:54PM D26.00009 Path integral studies of methane rotations in 4He clusters$^1$ , NIKOLAY MARKOVSKIY, CHI MAK, University of Southern California — Path integral simulations have been carried out to study the rotations of a methane inside a single shell of 4He atoms at 0.3 K to address the question of whether dopant molecule rotations can be used to probe the quantum statistics and superfluidity of the shell. We examined the effects of the probe molecule on the 4He exchanges and their counter effects on the renormalized rotation constant of the probe systematically by varying the intrinsic moment of inertia of the methane. The observed effects show strong dependence on the intrinsic moment of inertia of the rotating probe, with a heavy probe favoring stronger templating of the 4He density and a corresponding suppression of exchanges in the shell, as well as a large renormalization in the probe’s effective rotation constant, while a light probe shows almost no effect on the shell density or the effective rotation constant. These results can be rationalized in terms of a rotational smearing effect and suggest that there is no clearly quantifiable relationship between the superfluid fraction of the shell and the renormalized rotation constant of the probe for cases where the probe molecule has weak anisotropic interactions with the 4He atoms.

$^1$National Science Foundation

5:06PM D26.00010 Pump-probe spectroscopy of Rg-Br$_2$ linear isomers$^1$ , JORDAN PIO, CRAIG BIELER, WYTZE VAN DER VEER, KENNETH JANDA, University of California-Irvine — We have recorded and analyzed the $X$—$B$ spectra for three Rg–Br$_2$ linear isomers [Rg = He, Ne, Ar] using pump-probe spectroscopy. This work is an interesting test case for the transition from quantum to quasi-classical dynamics, and how the dynamics are interconnected with changes in the potential energy surface. Helium is not only much lighter than argon, but the He–Br$_2$ potential well is much shallower than that of Ar–Br$_2$. Excitation spectra to individual Rg–Br$_2$ (B, $\nu$) intermolecular potentials were recorded by probing the Br$_2$ (B, $\nu$) asymptotic limit of the potential while scanning the pump laser. The continuum spectra of the three species are very different, with the He–Br$_2$ spectrum peaking at threshold while the Ar–Br$_2$ spectrum is negligible at threshold and strongly blue shifted. The linear Ne–Br$_2$ bond energy was measured to be 71 ± 3 cm$^{-1}$ by the threshold energy for the onset of the continuum. Since excitation tends to move electron density to the $\nu^*$ orbital of the Br–Br bond near the rare gas atom, the intramolecular stretching vibration (Br–Br) and the intermolecular stretching vibration (Rg–Br) are strongly coupled. The experiments will be compared to a two dimensional model using the best available potential energy functions.

$^1$Supported by NSF Award Nos. CHE-0213149 and CHE-0404743.
delta M plots indicating an increase in the switching field distribution. This work was supported by NSF Grant# DMR-0302544.

exhibit a negative delta M curve indicative of magnetostatic interactions. As the inter-wire spacing increases there is a broadening of the dipolar component of the diameter of nanowires from 30 to 188 nm, the magnetic easy axis switches from perpendicular to parallel to the nanowire’s major axis. This is further exhibit the hexagonal closed packed polycrystalline structure. The direction of the magnetic easy axis is controllable as a function of wire diameter. By increasing recording, sensors and other electronic devices. The magnetic properties of nanowires are determined by the competition between magnetocrystalline and

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CoFe


SANS experiment observes the convolution of the nuclear and magnetic terms, we have implemented and further developed an algorithm to separate the four spin are described elsewhere [1]. An FeSi supermirror polarized the incident neutrons, and a polarized 3He cell was used as a spin analyzer. While a typical magnetic of the magnetic interparticle correlations. These particles were 7 nm in diameter with an average edge-to-edge separation of 2.5 nm. Preparation techniques studied ferromagnetic magnetite monodisperse nanospheres in order to determine the field (0 and 1.3 Tesla) and temperature (50, 100, and 200 K) dependence of the magnetic interparticle correlations. These particles were 7 nm in diameter with an average edge-to-edge separation of 2.5 nm. Preparation techniques are described elsewhere [1]. An FeSi supermirror polarized the incident neutrons, and a polarized 3He cell was used as a spin analyzer. While a typical magnetic SANS experiment observes the convolution of the nuclear and magnetic terms, we have implemented and further developed an algorithm to separate the four spin dependent cross sections. This provides an unambiguous separation and measurement of magnetic and nuclear contributions. At low temperatures, magnetic correlation lengths have been found to be significantly larger than at high temperatures.


2:42PM D27.00002 Artificial Nanomagnet with Lateral Confinement . LIFENG YIN, NOPPI WIDJAJA, JIAN SHEN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — For artificially low dimensional nanodots, the exchange interaction and dipole-dipole magnetostatic interaction can no longer stabilize the long range magnetic order at finite temperature. However, the electron-mediated indirect exchange interaction could be enhanced at surfaces due to the symmetry broken. A collective ferromagnetic behavior in two-dimensional Fe dot assemblies grown on a single crystal Cu(111) surface has been reported[1]. These Fe nanodots were grown using a novel method called buffer-layer assisted growth. The ferromagnetic ordering temperature appears to depend not only sensitively on the average spacing between the dots, but also strongly associated with the presence of surfaces states. The vicinal surfaces have been found a rich variety of novel behavior that results from broken translational symmetry by surface atomic steps. The presence of a free-electron-like Shockley surface state on the corresponding flat Cu(111) surface will be interrupted on vicinal surface. More interestingly, a switch between two qualitatively different regimes at a miscut of 7° takes place[2]. In this work, a curve-polished Cu(111) (0-8° miscut) substrate is used to tune the surface electronic states, and in turn influences the electron-mediated indirect exchange interaction of Fe nanodots. [1] J. P. Pierce et al., Phys. Rev. Lett. 92, 237201 (2004). [2] J.E. Ortega et al., Phys. Rev. Lett. 84, 6110 (2000).

2:54PM D27.00003 Magnetic Correlations In A Magnetite Nanoparticle Assembly Investigated Using Polarized SANS . KATHRYN KRYCKA, NCNR, NIST, CHARLES HOGLE, Carnegie Mellon University. YUMI IJIRI, Oberlin College. RYAN BOOTH, Carnegie Mellon University. JULIE BORCHERS, WANGCHUN CHEN, MARK LAVER, THOMAS GENTILE, BRIAN MARANVILLE, NCNR, NIST, BENJAMIN BRELSLAUER, SARA MAJETIC, Carnegie Mellon University — Using small angle neutron scattering (SANS) with polarization analysis, we have studied ferromagnetic magnetic monodisperse nanoparticles in order to determine the field (0 and 1.3 Tesla) and temperature (50, 100, and 200 K) dependence of the magnetic interparticle correlations. These particles were 7 nm in diameter with an average edge-to-edge separation of 2.5 nm. Preparation techniques are described elsewhere [1]. An FeSi supermirror polarized the incident neutrons, and a polarized 3He cell was used as a spin analyzer. While a typical magnetic SANS experiment observes the convolution of the nuclear and magnetic terms, we have implemented and further developed an algorithm to separate the four spin dependent cross sections. This provides an unambiguous separation and measurement of magnetic and nuclear contributions. At low temperatures, magnetic correlation lengths have been found to be significantly larger than at high temperatures.


3:06PM D27.00004 Magnetic Nanocheckerboards with Tunable Sizes in the Mn-Doped CoFe₂O₄ Spinel . CHENGLIN ZHANG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, C.M. TSENG, C.H. CHEN, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, S. YEO, Y.J. CHOI, S.W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — In the Mn-doped CoFe₂O₄ spinel, a highly ordered array of two types of rectangular nanorods, ~300 nm in length and a few nanometer in size, is achieved through chemical phase separation mediated by cooperative Jahn-Teller distortions. At room temperature, the magnetic nanorods with composition close to CoFe₂O₄ interlace with the paramagnetic counterpart and form a highly organized checkerboard pattern in the cross section. The checkerboard size, varying in the range of ~3 nm and ~80 nm, is tunable with composition as well as with the isothermal annealing time This may be of potential significance to the next generation magnetic storage. The magnetic nanocheckerboards exhibit a nearly ideal configuration for perpendicular recording media.

3:18PM D27.00005 Magnetic interactions among Co nanowires . HAFSA KHURSHID, MICHAEL BONDER, GEAROGE HADJIPANAYIS, University of DE — Magnetic nanowires have recently gained much attention because of their potential applications in magnetic recording, sensors and optoelectronic devices. The magnetic properties of nanowires are determined by the competition between magnetocrystalline and shape anisotropy resulting from the reduced dimensionality of the system. In this study we present results on the magnetic interactions among arrays of electrodeposited Co nanowires as a function of inter-wire spacing and nanowire diameter. X-Ray diffraction and electron microscopy reveal that the nanowires exhibit the hexagonal closed packed polycrystalline structure. The direction of the magnetic easy axis is controllable as a function of wire diameter. By increasing the diameter of nanowires from 30 to 188 nm, the magnetic easy axis switches from perpendicular to parallel to the nanowire’s major axis. This is further evidenced by a decrease in coercivity from 1200 to 100 Oe and a reduced loop squarness. The magnetic interactions were probed using delta M plots. All samples exhibit a negative delta M curve indicative of magnetostatic interactions. As the inter-wire spacing increases there is a broadening of the dipolar component of delta M plots indicating an increase in the switching field distribution. This work was supported by NSF Grant# DMR-0302544.
studied the magnetic properties of face-centered-cubic (fcc) Co nanoparticles made by the cluster gun. The zero field-cooled (ZFC) and field-cooled (FC) $M(T)$ curves at different fields show that the blocking temperature is shifted to lower temperature when the applied magnetic field is increased. This behavior could be due to a decreased energy barrier at increased filed or to inter-particle dipole-dipole interactions. $M$ vs $H/T$ data above the blocking temperature show that the latter might be responsible for this behavior. The dynamics of the FC magnetization were also studied. The $M(T)$ curves on FC samples obtained with the magnetic field on and off at different temperatures, show that the sample remembered its thermal history and demonstrated a memory effect at temperatures lower than the blocking temperature. However, this memory effects were not observed in the ZFC samples. The magnetic relaxation with a change at low temperature also shows a memory effect at temperature below the blocking temperature. The $M(T)$ curves at different fields and memory effects indicate that the dynamics of nanoparticles are due to the distribution of particle sizes and inter-particle interactions. Work Supported by NSF GRANT # DMR-0302544.

In this work we have studied the magnetic properties of face-centered-cubic (fcc) Co nanoparticles made by the cluster gun. The zero field-cooled (ZFC) and field-cooled (FC) $M(T)$ curves at different fields show that the blocking temperature is shifted to lower temperature when the applied magnetic field is increased. This behavior could be due to a decreased energy barrier at increased filed or to inter-particle dipole-dipole interactions. $M$ vs $H/T$ data above the blocking temperature show that the latter might be responsible for this behavior. The dynamics of the FC magnetization were also studied. The $M(T)$ curves on FC samples obtained with the magnetic field on and off at different temperatures, show that the sample remembered its thermal history and demonstrated a memory effect at temperatures lower than the blocking temperature. However, this memory effects were not observed in the ZFC samples. The magnetic relaxation with a change at low temperature also shows a memory effect at temperature below the blocking temperature. The $M(T)$ curves at different fields and memory effects indicate that the dynamics of nanoparticles are due to the distribution of particle sizes and inter-particle interactions. Work Supported by NSF GRANT # DMR-0302544.

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In this work we have studied the magnetic properties of face-centered-cubic (fcc) Co nanoparticles made by the cluster gun. The zero field-cooled (ZFC) and field-cooled (FC) $M(T)$ curves at different fields show that the blocking temperature is shifted to lower temperature when the applied magnetic field is increased. This behavior could be due to a decreased energy barrier at increased filed or to inter-particle dipole-dipole interactions. $M$ vs $H/T$ data above the blocking temperature show that the latter might be responsible for this behavior. The dynamics of the FC magnetization were also studied. The $M(T)$ curves on FC samples obtained with the magnetic field on and off at different temperatures, show that the sample remembered its thermal history and demonstrated a memory effect at temperatures lower than the blocking temperature. However, this memory effects were not observed in the ZFC samples. The magnetic relaxation with a change at low temperature also shows a memory effect at temperature below the blocking temperature. The $M(T)$ curves at different fields and memory effects indicate that the dynamics of nanoparticles are due to the distribution of particle sizes and inter-particle interactions. Work Supported by NSF GRANT # DMR-0302544.
4:54PM D27.00013 Growth of Co nanoclusters on rutile TiO2 (110) surface1, EN CAI, XUEWEN WANG, JIANDI ZHANG, Florida International University — Fabrication of magnetic nanodots with uniform size and density is one of the key issues of studying the structure and property of a nanomagnet system. We report here our studies on the growth of Co nanoclusters on rutile TiO2 (110) surface. Well ordered TiO2 (110) surface is prepared in the UHV chamber via Ar+ sputtering and annealing. Co deposition is carried out in situ by molecular beam epitaxy and characterized with STM. Growth parameters are tuned to optimize the uniformity of dot size and density. Co dot coverage, size and density are investigated as functions of deposition rate and time as well as post-annealing temperature. Our results show that uniformity of the dots mainly depends on deposition rate, and the density if the dots primarily depends on the coverage of the dots, while the size of the dots mainly depends on the deposition rate and post-annealing temperature instead of coverage. Growth mechanism will be discussed.

5:06PM D27.00014 Tuning of the magnetocrystalline anisotropy in CoFe3−xO4 nanoparticles through cobalt doping1, RONALD TACKETT, SUDAKAR CHANDRAN, RATNA NAIK, GAVIN LAWES, Wayne State University, CORNELIU RABLAU, PREM VAISHNAV, Kettering University — We report on the effect of cobalt doping on the magnetocrystalline anisotropy of CoFe3−xO4 nanoparticles. The CoFe3−xO4 (0 ≤ x ≤ 0.15) nanoparticles were synthesized through the co-precipitation of ammonium hydroxide in an environment of Fe2+, Fe3+, and varying concentrations of Co2+. The size and crystallinity were confirmed using transmission electron microscopy, with a mean size of 17 ± 4 nm which was found to be constant across the different cobalt dopings. The magnetic properties were investigated through the use of dc and ac magnetic susceptibility, with the effective magnetocrystalline anisotropies being extracted from these data. The effective magnetocrystalline anisotropy found from each method were, within acceptable experimental error, found to agree, as well as increase linearly with cobalt doping. The effective anisotropy values were found to increase in magnitude by 100% as the cobalt fraction was increased from x = 0 to x = 0.1. This trend allows for the tuning of the magnetic isotropy of iron oxide nanoparticles through cobalt doping.

5:18PM D27.00015 Preparation of cobalt-ferrite nanoparticles within a biopolymer template1, MARCO GARZA, VIRGILIO GONZÁLEZ, ALEJANDRO TORRES-Castro, MOISÉS HINOJOSA, UBALDO ORTIZ, UANL-FIME — Using an in-situ co-precipitation reaction from solid dissolutions of stoichiometric amounts of Fe (III) and Co (II) inorganic salts, it was prepared highly loaded nanocomposites (as high as 75% w/w) of cobalt-ferrite nanoparticles within a chitosan matrix, with particle size of about 7 nm, narrow particle size distribution and superparamagnetic character. Nanoparticle samples were characterized by high resolution transmission electron microscopy (HRTEM), UV-vis spectrometry and magnetic measurements by SQUID, using magnetization-field dependent, M(H), and magnetization-temperature dependent, M(T), studies.

1Supported by NSF-DMR0346826.

Monday, March 10, 2008 2:30PM - 5:30PM

Session D28 DMP: Focus Session: Transport in Nanostructures III: Single Molecules Morial Convention Center 220

2:30PM D28.00001 Understanding the Conductance of Single-Molecule Junctions from First Principles1, SU YING QUEK, Molecular Foundry, Lawrence Berkeley National Laboratory — Discovering the anatomy of single-molecule junctions, in order to exploit their transport behavior, poses fundamental challenges to nanoscience. First-principles calculations based on density-functional theory (DFT) can, together with experiment, provide detailed atom-scale insights into the transport properties, and their relation to junction structure and electronic properties. Here, a DFT scattering state approach [1] is used to explore the single-molecule conductance of two prototypical junctions as a function of junction geometry, in the context of recent experiments. First, the computed conductance of 15 distinct benzene-diamine-Au junctions is compared to a large robust experimental data set [2]. The amine-gold bonding is shown to be highly selective, but flexible, resulting in a conductance that is insensitive to other details of the junction structure. The range of computed conductance corresponds well to the narrow distribution in experiment, although the average calculated conductance is approximately 7 times larger. This discrepancy is attributed to the absence of many-electron corrections in the DFT molecular orbital energies; a simple physically-motivated estimate for the self-energy corrections results in a conductance that is much closer to experiment [3]. Second, similar first-principles techniques are applied to a range of bipyridine-Au junctions. The extent to which Au-pyridine link bonding is affected by the constraints of forming bipyridine-Au junctions is investigated. In some contrast to the amine case, the computed conductance shows a strong sensitivity to the tilt of the bipyridine rings relative to the Au surfaces. Experiments probing the conductance of bipyridine-Au junctions are discussed in the context of these findings. [1] H. J. Choi et al, Phys Rev B, 76, 155420 (2007) [2] L. Venkataraman et al, Nano Lett 6, 458 (2006) [3] S. Y. Quek et al, Nano Lett. 7, 3477 (2007)

1This work is supported by DOE (DE-AC02-05CH11231).

3:06PM D28.00002 Single Molecule Conductance and Contact Chemistry, LATHA VENKATARAMAN, YOUNG PARK, ADAM WHALLEY, MASHÁ KAMENETSKA, MICHAEL STEIGERWALD, COLIN NUCKOLLS, MARK HYBERTSEN, Columbia University — Our previous experiments probing the conductance of single molecule circuits with amine-gold linkages have demonstrated the relationship between the electrical characteristics and the intrinsic molecular properties such as their length, conformation, gap between the highest occupied and lowest unoccupied molecular orbitals and the alignment of these levels to the metal Fermi level. Here we study different chemical linker groups expected to form donor-acceptor bonds to gold. We measure transport through single molecule junctions by repeatedly forming and breaking Au point contacts with a modified STM in a solution of the molecules terminated by Amine, Dimethyl Phosphine and Methyl Sulfide linker groups. The clear molecular signatures allow us to demonstrate a systematic dependence the link group.

3:18PM D28.00003 Conductance Trends in Single Molecule Junctions Formed Using Donor-Acceptor Links: Theoretical Analysis1, MAX B. KOENTOPP, LATHA VENKATARAMAN, MICHAEL L. STEIGERWALD, Columbia University, MARK S. HYBERTSEN, Brookhaven National Laboratory — The conductance of single molecule junctions using amine-gold links has been understood based on formation of a donor-acceptor bond involving the N lone pair and the s-orbital on an undercoordinated Au site on the electrode. Experiments probing junctions formed with alkanes terminated by dimethyl phosphines and methyl sulfides also show an unambiguous conductance signature. The structure and bonding in these junctions is analyzed using density functional theory based calculations. Like the amine link, the dimethyl phosphine and methyl sulfide bond to an under-coordinated Au site through a donor-acceptor motif. While the bond energy for the amine and methyl sulfide links are similar (0.6 eV), the dimethyl phosphine is significantly stronger (1.2 eV). Trends in measured junction conductance (amine < sulfide < phosphine) are analyzed in terms of available electronic channels.

1This work is supported by the NSF, NYSTAR and the DOE.
3:30PM D28.00004 Molecular Conductance of oligophenylene-vinylene in Metallic Break-Junctions

PATRICK WHEELER, MENG LU, DAVID CORLEY, JAMES TOUR, DOUG NATELSON, Rice University — Break junctions between a metallic tip and a metallic substrate have proven to be extremely useful tools for characterizing single-molecule electrical conductance. Conductance measurements while repeatedly breaking and reforming junctions are conducive to rapid statistical characterization. We will present preliminary results of room temperature break junction conductance measurements on amine-terminated oligophenylene-vinylene (OPV) oligomers. Recent low temperature measurements of OPV oligomers in the electromigrated gap configuration imply a large renormalization downward of the HOMO-LUMO gap. Since the HOMO-LUMO gap is correlated with the conductance and the tunneling coefficient, beta, break junction measurements should provide clarification about the HOMO-LUMO gap in these molecules.

3:42PM D28.00005 Probing mechanisms of electrical conduction in single organic molecules

LYUDMYLA ADAMSKA, IVAN OLEYNIK, University of South Florida, MORTKÖ KOZHUSHNER, Institute of Chemical Physics, RAS — The electrical conduction of relatively long (1-2 nm) single organic molecules occurs via resonant tunneling of charge carriers, electrons and/or holes, through the energy levels of negative molecular ion (electrons) and/or positive molecular ion (holes). The position of these resonant energy levels with respect to the Fermi levels of the anode and cathode determines the relative contributions of electron and hole conduction to the resonant current. These resonant levels depend on the applied bias, and are also influenced by several physical factors such as the polarization of the molecule, image potential and metal/molecule interfaces that are difficult to control under conditions of real experiment. In this presentation we suggest a method of unambiguous experimental determination of specific type of the conduction mechanism (electron or hole conduction) which is based on the idea of utilizing experimental techniques of nanocalorimetry.


MARC KAMENETSKA, Department of Applied Physics and Applied Math, Columbia University, MICHAEL FREI, MARC HYBERTSEN, CFN, Brookhaven National Laboratory, LATHA VENKATARAMAN — We measure the conductance of single molecules attached to gold electrodes by repeatedly forming and breaking Au point contacts with a modified STM in a solution of molecules. Conductance traces measured while pulling the point-contacts reveal steps due to the formation of single molecule junctions which can be elongated without a significant change in junction conductance. To better understand the mechanical stability of these single molecule junctions, we analyze data sets of 20000 or more individual conductance traces for a series of diamin molecules, measuring the distance over which junctions can persist. We find that the distance that a junction can be pulled is affected by the metal-molecule binding energy. In addition, we see an unambiguous relationship between geometry and stability, where both the length of the molecule as well as the atomic configuration of the contact electrode affect the distance over which a junction can persist.

4:06PM D28.00007 Tunneling Transport through Long Molecular Chains

EMIL PRODAN, Department of Physics, Yeshiva University, New York, NY, ROBERTO CAR, Chemistry Department, Princeton University, Princeton, NJ — The Riemann structure of the bands and other properties of the evanescent Bloch functions have been used to derived an asymptotic expression for the tunneling conductance through long molecular chains. Our results give the contact conductance in terms of an overlap integral of three well defined and physically relevant quantities. In particular, this formula shows how the conducting states of the leads couple to the evanescent Bloch functions of the insulating chain. The theory is applied to amine-linked alkyl and aromatic chains and the results are compared with the experiment. Using these applications, we discuss the key aspects and advantages of the theory. Extensions to spin dependent transport will be also discussed.

1Supported by NSF-MRSEC program through the Princeton Center for Complex Materials (PCCM), grant DMR 0213706, and by DOE through grant DE-FG02-05ER46201

4:18PM D28.00008 Transport properties of molecular wires from ab initio calculations

KENJI HIROSE, NEC Corp., NOBUHIKO KOBAYASHI, Univ. of Tsukuba — Understanding of electron transport through nanostructures becomes important with the advancement of fabrication process to construct atomic-scale devices. Due to the drastic change of transport properties by contact conditions to electrodes in local electric fields, first-principles calculation approaches are indispensable to understand and characterize the transport properties of nanometer-scale molecular devices. Here we focus on the transport properties of molecular wires bridged between metallic electrodes, especially on the effects of contacts to electrodes and on the dependence of the length of molecular wires on transport properties. We use an ab initio calculation method based on the scattering waves, which are obtained by the recursion-transfer-matrix (RTM) method, combined with non-equilibrium Green’s function (NEGF) method. We find that conductance shows exponential behaviors as a function of the length of molecular wires due to tunneling process determined by the HOMO-LUMO energy gap. From the voltage drop behaviors inside the molecular wires, we show that the contact resistances are well separated for the long molecular wires. We will present detailed data of electronic states at contacts to metallic electrodes under strong electronic fields and will discuss the polarization, screening effect, and potential barrier formation at contacts on the transport properties of molecular wires, comparing them with those of metallic atomic wires.

4:30PM D28.00009 The molecular electronics of protein fragments

DAVID CARDAMONE, GEORGE KIR-CZENOW, Simon Fraser University — Small fragments of polypeptide chains provide a uniquely scalable, customizable basis for nanoelectronic devices. Using a combination of ab initio and semi-empirical techniques, we arrive at a quantitative understanding of the charge transport properties of these molecules. This allows us to investigate their chemical and physical properties, such as lead-molecule bonding geometry, lead-induced distortion of molecular structure (e.g., molecular stretching), and device properties. We explain the observed current rectification in these molecules and further predict negative differential resistance, opening the way to protein-based nanoelectronic devices.

1This work was supported by NSERC, the Canadian Institute for Advanced Research, and Westgrid.

4:42PM D28.00010 Ab initio studies of electronic transport through amine-Au-linked junctions of photoactive molecules

DAVID A. STRUBBE, Dept. of Physics, University of California, Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory, SU YING QUEK, Molecular Foundry, LBNL, LATHA VENKATARAMAN, Dept. of Applied Physics, Columbia Univ., HYOUNG JOON CHOI, Dept. of Physics and IPAP, Yonsei Univ., J.B. NEATON, Molecular Foundry, LBNL, STEVEN G. LOUIE, Dept. of Physics, UC Berkeley, M.D. — Molecules linked to Au electrodes via amine groups have been shown to result in reproducible molecular conductance values for a wide range of single-molecule junctions [1,2]. Recent calculations have shown that these linkages result in a junction conductance relatively insensitive to atomic structure [3]. Here we exploit these well-defined linkages to study the effect of isomerization on conductance for the photoactive molecule 4,4'-diaminoazobenzene. We use a first-principles scattering-state method based on density-functional theory to explore structure and transport properties of the cis and trans isomers of the molecule, and we discuss implications for experiment. [1] L Venkataraman et al., Nature 442, 904-907 (2006); [2] L Venkataraman et al., Nano Lett. 6, 458-462 (2006); [3] SY Quek et al., Nano Lett. 7, 3477-3482 (2007).

1Support from DOE (DE-AC02-05CH11231), NSF (DMR07-05941 and IGERT Fellowship); computational resources from NERSC, TeraGrid.
4:54PM D28.00011 Electronic spectrum and orbital filling in a single-molecule junction. EDGAR A. OSORIO, KEVIN O’NEILL, Delft University of Technology, MAARTEN WEGEWIJS, RWTH Aachen, NICOLAI STUHR-HANSEN, JENS PAAKSE, THOMAS BJORNHOLM, University of Copenhagen, HERRE VAN DER ZANT, Delft University of Technology — We study single-electron tunneling in three-terminal devices in which a single molecule bridges the gap between source and drain electrode. The molecular devices are made by electromigration and at low temperatures excitations appear in the stability diagram. For the OPV-5 molecule more than fifteen different excitations are visible, of which twelve match Raman spectra and the remaining ones are due to vibrations of the molecule attached to gold electrodes at energies below 10 meV. Similar to carbon nanotubes, the observation of a singlet-triplet transition allow us to determine the orbital filling and spin configuration of the molecule.

5:06PM D28.00012 Gate effects on electronic transport in alkanedithiol single molecular junctions. HYUNWOO SONG, TAKHEE LEE, Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, YOUNGSANG KIM, HEEJUN JEE, Department of Applied Physics, Hanyang University — We investigate the gate effects on the electronic transport properties in alkanedithiol single molecular junctions. Using electromigration-induced break junction technique, we fabricated an array type of electrode pairs with nanometer-sized separation on top of naturally oxidized aluminum gate electrodes. The alkanedithiol molecules were bridged between the nanometer-sized gap that was achieved by breaking gold nanowires fabricated using electron-beam lithography with a controlled passage of current. The electric potential applied to the aluminum gate electrode shifts the molecular energy levels relative to the Fermi energy in the metallic contacts. We will discuss the gate-bias dependent current-voltage characteristics and other observed transport properties of alkanedithiol single molecular junctions in the off-resonant tunneling transport regime.

5:18PM D28.00013 Modeling of N@C$_{60}$ single-molecule transistors. CARSTEN TIMM, University of Kansas, JACOB E. GROSE, Cornell University, WOLFGANG HARNEIT, Free University Berlin, DANIEL C. RALPH, Cornell University — We report on recent experimental and theoretical results for single-molecule transistors involving endohedral N@C$_{60}$ fullerene molecules. In this talk, we will focus on the theoretical modeling. The observed differential conductance shows strong evidence for the exchange interaction between electrons in the fullerene LUMO and the nitrogen p-electrons, favoring an antiferromagnetic interaction. In addition, soft vibrational modes are seen, which are attributed to oscillations of the molecule as a whole. We discuss a model Hamiltonian that reproduces the main features of the experimental conductance.

Monday, March 10, 2008 2:30PM - 5:30PM
Session D29 DMP: Focus Session: Carbon Nanotubes and Related Materials IV: Graphene
Morial Convention Center 221

2:30PM D29.00001 Electronic properties of Dirac fermions in epitaxial graphene. SHUYUN ZHOU, UC Berkeley & LENL — Graphene, atomically thin layers of graphite, has attracted a lot of research interest because of its intriguing physics as well as its technological potential for next generation electronic devices. I will first present a detailed characterization of the growth of atomically thin films of epitaxial graphene on SiC, by using low energy electron microscopy (LEEM). The electronic properties of the films are hence studied by angle resolved photoemission spectroscopy (ARPES). Data as a function of doping, temperature and sample thickness are presented and the role of disorder and many body interactions will be discussed. Finally, the presence of a bandgap in the spectra of Dirac fermions will be presented and its potential for bandgap engineering will be discussed.

3:06PM D29.00002 Electronic Confinement in Epitaxial Graphene As Seen by ARPES. DAVID SIEGEL, SHUYUN ZHOU, Department of Physics, University of California; Berkeley/Materials Sciences Division, Lawrence Berkeley National Laboratory, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, ANDREAS SCHMID, FARID EL GABALY, Materials Sciences Division, Lawrence Berkeley National Laboratory — The growth of graphene on 6-H SiC and its electronic structure have been studied with low energy electron microscopy (LEEM) and angle-resolved photoemission spectroscopy (ARPES) respectively. Some of the critical growth parameters that determine sample homogeneity and domain properties have been identified. The resulting electronic structure presents features that generally agree with the conical dispersion of Dirac quasiparticles, however deviations are observed near the Dirac point energy. The dependence of these deviations on real-space electronic confinement is discussed.

3:18PM D29.00003 Tuning the phonon self-energy of a graphene bilayer. JUN YAN, ERIK HENRIKSEN, PHILIP KIM, ARON PINCUK, Columbia University — We use low temperature Raman spectroscopy and the electric field effect to investigate the coupling of long wavelength optical phonons (the G-band) with charge carriers in bilayer graphene. The charge tunable phonon spectra exhibit a remarkable symmetry which reflects the underlying particle-hole symmetry of the electron band structure. The change of phonon line-width is interpreted as a Landau damping of the phonon into resonant electron-hole pair transitions. The phonon energy exhibits an intriguing non-monotonic evolution with charge density. We found that the electron-hole pair excitation stiffness (softens) the lattice vibration when its energy is smaller (larger) than the phonon energy, in agreement with theoretical predictions for deformation electron-phonon coupling.

Support by ONR, NSF and DOE

3:30PM D29.00004 Graphene on a graphite surface: effect of interlayer coupling. ADINA LUICAN, GUOHONG LI, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — We present low temperature high magnetic field scanning tunneling microscopy and spectroscopy on a sheet of graphene suspended above a graphite substrate. The sheet consists of two regions that couple to the substrate with different strengths resulting in two distinct sequences of Landau Levels (LL). One region exhibits a sequence that reflects the underlying particle-hole symmetry of the electron band structure. The change of phonon line-width is interpreted as a Landau damping of the phonon into resonant electron-hole pair transitions. The phonon energy exhibits an intriguing non-monotonic evolution with charge density. We found that the electron-hole pair excitation stiffness (softens) the lattice vibration when its energy is smaller (larger) than the phonon energy, in agreement with theoretical predictions for deformation electron-phonon coupling.

4:06PM D29.00005 Scanning tunneling microscopy/spectroscopy studies of local electronic structure in Epitaxial Graphene. NIKHIL SHARMA, MICHAEL SPRINKLE, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology/ CNRS, France, WALTER DEHEER, PHILIP FIRST, Georgia Institute of Technology — Epitaxial growth of graphene on hexagonal SiC by thermal desorption of Si has produced high quality films, providing a potential route to wafer-scale graphene electronics. However, many aspects of this new electronic material system remain to be understood. Using scanning tunneling microscopy and spectroscopy (STM/STS), we investigate the layer-dependent effect of atomic defects and deposited metal islands on the local electronic structure of epitaxial graphene. Metal islands locally dope the graphene due to the work function difference between materials, and atomic defects can have a similar effect. The lateral gradient in carrier density and the possible transition from hole- to electron- doping (PN junction) is investigated experimentally for these cases.
3:54PM D29.00006 Transport in multilayered epitaxial graphene , CLAIRE BERGER, Georgia Tech-Atlanta and CNRS-France, XIAOSONG WU, MIKE SPRINKLE, XUEBIN LI, Georgia Tech-Physics, Atlanta, FAN MING, WALT DE HEER, Georgia Tech-Physics, Atlanta — We present recent results of electronic transport in multilayered epitaxial graphene (EG) grown by thermal decomposition of SiC wafers. Because of the rotational stacking of the layers, it was recently shown theoretically that the system should retain essentially the same band structure as single layer graphene. The system consists of a charged layer at the SiC/EG interface, as revealed by the period of the Shubnikov-de Haas oscillations (a few 10^{12}/cm^2), and quasi-neutral layers on top. We discuss possible effects of the multilayering in the transport properties, such as the large positive increase in field of the magnetoresistance $\rho_{xx}$, the weak amplitude of the Shubnikov-de Haas and the overall features of the Hall effect, in particular the anomaly of the Hall resistance $\rho_{xy}$ observed at low field.

4:06PM D29.00007 Electronic compressibility of a graphene bilayer , SILVIA VIOLA KUSMINSKYI, Boston University, JOHAN NILSSON, Boston University and Leiden University, DAVID CAMPBELL, ANTONIO CASTRO NETO, Boston University — We calculate the electronic compressibility arising from electron-electron interactions for a graphene bilayer within the Hartree-Fock approximation. We show that, due to the chiral nature of the particles in this system, the compressibility is rather different from either of the two-dimensional electron gas or ordinary semiconductors. We find that an inherent competition between the contributions coming from intra-band exchange interactions (dominant at low densities) and inter-band interactions (dominant at moderate densities) leads to a non-monotonic behavior of the compressibility as a function of carrier density.

4:18PM D29.00008 Charge inhomogeneity in a single and bilayer graphene , HARI DAHAL, Boston College, TIM WEHLING, University of Hamburg, KEVIN BEDELL, Boston College, JIAN-XIN ZHU, ALEXANDER BALATSKY, Los Alamos National Laboratory — We study the possibility of charge ordered state in both single and bilayer graphene using a real space tight binding model. We find that the single layer graphene always remains in a liquid phase; the reason being the higher kinetic energy compared to the potential energy. The bilayer graphene on the other hand can have an inhomogeneous distribution of the charge, namely the charge density wave (CDW) state. The CDW state is commensurate with the lattice. The charge ordered state is stabilized by the Coulomb interaction of the carriers of two layers. We also predicted a kinetic energy driven (KID) inhomogeneous phase. This phase can be stabilized by the inter layer hopping energy. The KID phase and the CDW phase compete with each other below the half filling whereas they cooperate above half filling. For the physical parameter of bilayer graphene CDW phase always wins over the KID phase. Hari P. Dahal, Tim O. Wehling, Kevin S. Bedell, Jian-Xin Zhu, Alexander V. Balatsky

3:30PM D29.00009 Interplay of Coulomb interactions and rippling of monolayer graphene: RG approach , OSKAR VAFEK, NHMFL and FSU, VLADIMIR JURICIC, IGOR HERBUT, Simon Fraser University — The effects of electron-electron Coulomb interactions and rippling disorder of a mono-layer graphene are studied at half-filling using renormalization group. It is found that the system flows to an infra-red stable line of fixed points which is accessible perturbatively and along which the zero temperature minimal metallic conductivity is non-universal and enhanced relative to the clean non-interacting fixed point. An estimate of the typical random vector potential representing ripples in graphene brings the theoretical real value of the minimal conductivity into the vicinity of $4e^2/h$.

4:42PM D29.00010 Graphene in a magnetic field and a superlattice potential, J.M.B. LOPES DOS SANTOS, CFP and Dept. Fisica, Faculdade de Ciencias, Universidade do Porto, N.M.R. PERES, Centro de Fisica e Dept. Fisica, Universidade do Minho, A.H. CASTRO NETO, Physics Department, Boston University — The problem of electrons in a periodic potential in the presence of a magnetic field is revisited here in the context of graphene, by considering a superlattice periodic perturbation on the Dirac-Weyl equation for massless fermions. We solve the problem of a periodic potential for massless Dirac Fermions in a magnetic field. The relevance for graphene physics arises from the possibility of a superlattice modulation, both in single-layer graphene, due to the substrate, and in few layer graphene due to rotational stacking faults, which give rise to long wavelength moire patterns [1,2].

1 JMBLS and NMRP acknowledge financial support from project PTDC/FIS/6440/2006.

4:54PM D29.00011 Quenching of quantum Hall effect and the role of undoped planes in epitaxial graphene, PIERRE DARANCET, NICOLAS WIPF, DIDIER MAYOU, Institut NEEL CNRS/UJF, 25 rue des Martyrs BP166, 38042 Grenoble — We propose a mechanism for the quenching of the Shubnikov de Haas oscillations and the quantum Hall effect observed in epitaxial graphene. This involves a coupling between the uncharged rotationally stacked layers and the charged graphene layer at the interface. In a magnetic field, the extraordinary graphene Fermi level leads to that Mott’s relation holds at low temperature. For higher temperatures, there are strong deviations due to the linear density of states. For strong impurity scattering, near the unitary limit, the formation of a band of impurity states near the Fermi level is unavoidable, and the Mott’s relation is violated. The relevance for graphene physics arises from the possibility of a superlattice modulation, both in single-layer graphene, due to the substrate, and in few layer graphene due to rotational stacking faults, which give rise to long wavelength moire patterns [1,2].


2 JMB Lopes dos Santos, NMR Peres and AH Castro Neto, arXiv:0704.2128v1 [cond-mat.mtrl-sci]

5:06PM D29.00012 Anomalous Thermoelectric Effect in Graphene, TOMAS LOFWANDER, MIKAEL FOGELSTROM, Chalmers University of Technology — We present calculations of the thermal and electric linear response in graphene, including disorder in the self-consistent t-matrix approximation [1]. For strong impurity scattering, near the unitary limit, the formation of a band of impurity states near the Fermi level leads to that Mott’s relation holds at low temperature. For higher temperatures, there are strong deviations due to the linear density of states. The low-temperature thermopower is proportional to the inverse of the impurity potential and the inverse of the impurity density. Information about impurity scattering in graphene can be extracted from the thermopower, either measured directly, or extracted via Mott’s relation from the electron-density dependence of the electric conductivity.


5:18PM D29.00013 Charge Carrier Interaction with a Purely Electronic Collective Mode: “Plasmarons” and the Infrared Response of Semi-metal Bismuth, P. PETER ARMITAGE, The Johns Hopkins University, RICCARDO TEOIDOSI, IN ENRICO GIANNINI, University of Geneve, LASZLO FORRO, Ecole Polytechnique Federale de Lausanne, DIRK VAN DER MAREL, University of Geneve — We present a detailed pressure and temperature dependent optical study of single-crystal bismuth using infrared reflectivity and ellipsometry. In the ambient pressure optical conductivity, an anomalous temperature dependent mid-infrared absorption feature is observed. An extended Drude model analysis reveals that it can be connected to a sharp upturn in the scattering rate, the frequency of which exactly tracks the strongly temperature dependent plasmon frequency. We interpret this absorption and increased scattering as direct optical evidence for a charge carrier interaction with a collective mode of purely electronic origin, here electron-plasmon scattering. The observation of a “plasmaron” as such is made possible by the exceptional properties of semi-metallic bismuth, but it is also likely relevant to the low energy transport and thermodynamic properties of other semi-metals, like graphite and graphene. As a function of pressure, we observe massive changes in bismuth’s optical and infrared conductivity as the material approaches a Lifshitz-like metal/insulator transition.
2:30PM D30.00001 Electrical, Mechanical, and Optical Studies of Carbon Nanotubes of Known Chiral Index. JAMES HONE, Columbia University — Because small changes in the crystal structure (chirality) of carbon nanotubes can produce large changes in their electrical properties, it is important to understand the relationship between structure and transport properties, both for basic science and for applications. We have developed a unique set of tools for characterizing and manipulating nanotubes that allow for detailed studies of the properties of known-chirality nanotubes. Completed and ongoing studies include: structure-correlated optical properties; tube-tube interactions; variable electron-phonon coupling; electromechanical properties; structure-correlated electrical transport; nanotube intermolecular heterojunctions; and mechanical stiffness and strength.

2:30PM D30.00002 Electron field emission from Carbon Nanotube Composites: Transport and Local Electric Fields. DAVID CAREY, THOMAS CONNOLLY, RICHARD SMITH, University of Surrey, JONATHAN COLEMAN, Trinity College Dublin — Electron field emission characterisation of carbon nanotube polymer composites has been performed where emission at low nanotube mass fractions (<10%) has been observed. Nanotubes have been embedded in two different types of polymer: PmPV, a conjugated polymer and PVA, polyvinyl alcohol. It is shown that for nanotubes embedded in PmPV, the field emission is strongly influenced by charge transport through the film. For nanotubes in PVA a transition from bulk transport to a Fowler-Nordheim emission mechanism is seen as the mass fraction exceeds about 1-2%. Estimates of the local field as a function of mass fraction are also shown. The potential role of nanotube — polymer composites produced by solution processing to large area cathodes with a controllable mass fraction will be discussed.

3:18PM D30.00003 Metal-Semiconductor-Metal (MSM) Photodetectors with Single-walled Carbon Nanotube Film Schottky Electrodes on GaAs. ASHKAN BEHNAM, JASON JOHNSON, YONGHO CHOI, LEILA NORIEGA, University of Florida, GÜNHAH ERTOSUN, Stanford University, ZHJANGCHUN WU, ANDREW RINZLER, University of Florida, PAVAN KAPUR, KRISHNA SARASWAT, Stanford University, ANT URAL, University of Florida — We fabricate and experimentally characterize the dark and photocurrent in metal-semiconductor-metal (MSM) photodetectors with transparent and conductive single-walled carbon nanotube (CNT) film electrodes on GaAs. The dark current measurements of MSM structures reveal that the CNT film forms a Schottky contact on GaAs substrates. The Schottky barrier height and the CNT film workfunction are extracted to be approximately 0.85 and 4.6 eV, respectively, based on dark current measurements as a function of temperature. We also study the effect of device geometry on the dark current of the CNT film-GaAs MSM devices. Furthermore, we find that CNT film MSM devices exhibit a significantly lower dark current and higher normalized photo-to-dark current ratio compared to metal control samples. We explain these observations by comparing the interfaces in these structures. This work opens up the possibility of integrating CNT films as Schottky electrodes in conventional semiconductor electronic and optoelectronic devices.

3:30PM D30.00004 Anomalous Coulomb oscillation in crossed carbon nanotubes. SEUNG JAE BAEK, Nano Systems Institute-National Core Research Center, Seoul National University, DONGSU LEE, Department of Physics and Astronomy, Seoul National University, SEUNG JOO PARK. Nano Systems Institute-National Core Research Center, Seoul National University, YUNG WOO PARK, Department of Physics and Astronomy, Seoul National University, JOHANNES SVENSSON, Department of Physics, Gothenburg University, SE-41296 Gothenburg, Sweden, MATS JONSON, Department of Physics, Gothenburg University, SE-41296, Sweden, ELEANOR E. B. CAMPBELL, Department of Physics, Gothenburg University, SE-41296 Gothenburg, Sweden — Single-walled carbon nanotube (SWCNT) crossed junctions separated by an insulating layer were fabricated to investigate the double quantum dot modulated by a single gate (DQD-sg). Anomalous Coulomb oscillations were observed on the lower CNT at low temperature, where the behavior was interpreted by the concept of a double quantum dot (DQD) system http://scitation.aip.org/getabs/servlet/GetabsServlet?prog=normal&id =APPLAB000089000023233107000001&itid=cpsv&gifs=yes [1]. To understand it more clearly, we have intentionally fabricated crossed CNTs without oxide layer in between. The observed anomalous Coulomb oscillations indicate that the contact resistance between the two tubes becomes a potential barrier splitting the initial single QD into the DQD, and the back-gate modulates the energy levels of the DQD.

3:42PM D30.00005 Strain Tuning of the Photocurrent Spectrum in Single wall Carbon Nanotubes. PRASANTH GOPINATH, A. MOHITE, H. SHAH, J. LIN, B. NAGABHIRAVA, T. BANSAL, B. ALPHENAAAR, University of Louisville — The electronic structure of a single-wall nanotube (SWNT) can be substantially modified by the application of uniaxial strain. We use displacement photocurrent spectroscopy to study the effect of uniaxial strain on the optical transitions of a SWNT in the energy range 0.5eV-3eV. This broad energy range allows us to compare the strain dependence of the lowest (E11) and higher order (E22 and E33) optical transitions of semiconducting SWNT’s. As predicted by a simple non-interacting model, we observe an energy shift of each transition with increasing strain. By fitting the model to the magnitude and slope of the energy shift for the lowest energy transition (E11) the nanotube chirality can be identified uniquely. For the higher energy transitions, the data deviates significantly from the non-interacting model, presumably because of the influence of the excitonic binding energy. Finally, we observe a large reversible increase in the magnitude of the photocurrent around the ground state (E11) energy regime with an applied strain of 0.01%. We attribute this to reversible strain induced defect states opening up within the bandgap of the SWNT.

3:54PM D30.00006 Negative magneto resistance in carbon nanotubes: A first principle study. LI CHEN, SAROJ NAYAK — We have studied spin transport through single wall carbon nanotube (SWNT) with nickel contacts using ab initio density functional theory and green’s function based Landauer Büttiker formalism. Our results show enhanced current for anti-parallel alignment compared to that obtained for parallel alignment. This non Julliérè’s model results due to finite size effect and this talk will present a detailed atomic level mechanism of such phenomena. Our results will be discussed in the light of recent experimental studies.
Lowell — We present a model to characterize ensembles of NT networks using properties of individual from measurement and from ab initio computations, and MEG NOAH, YOUNG-KYUN KWON, Nanomanufacturing Center of Excellence and Center for High-rate Nanomanufacturing, University of Massachusetts.

Using this technique we are then able to both image with diffraction-limited resolution and electrically characterize up to hundreds of CNTs rapidly in the displays gate dependence similar to that of overall conductance of the CNT, allowing us to probe the local electronic properties of the CNT simultaneously.

1 nanotubes (CNTs) is a painstaking and time-consuming process, requiring a serial study of individual CNT devices. We present a novel method utilizing a Fourier-transform spectrometer and microscope to induce currents in electrically biased nanotubes. This approach enables the rapid acquisition of high-resolution photocurrent spectra near the bandgap of the larger diameter (> 1.7 nm) nanotubes commonly produced by synthesis using chemical vapor deposition. We have recorded optical transitions with energies as low as 0.4 eV for individual nanotubes. The structures used in these measurements consisted of isolated nanotubes with well-separated metal contacts on a Si back gate. In addition to describing the experimental approach and results, we will discuss the sensitive dependence of the measured photocurrent on the electrical biasing conditions.

Our goal is to optimize nanomanufacturing parameters like channel size for a user-defined application be it gas sensor, pressure actuator, or semiconductor and then compared subjected to different environmental conditions. Validation with experimental data resulting from inhomogeneous NT mixtures is presented.

We investigate the properties of single-walled carbon nanotubes in transverse electric and magnetic fields. We find via band structure calculations that these fields can break particle-hole symmetry as well as that of the two Dirac points. Additionally, the speed of the left and right movers is generally different in the presence of both electric and magnetic fields. We consider the effect of these fields on Coulomb interactions within the tube and show that they can be used to tune the interaction parameter K associated with the Luttinger liquid properties of the tube. Finally, we discuss finite size effects and Coulomb blockade physics for holes. We further show that SO coupling determines the filling order in the many-electron ground states, in a way different than that expected from electron-electron interactions. At low magnetic fields we find that the two-electron ground state is neither a spin-triplet nor a spin-singlet, but a Slater determinant with wave functions that are predominantly spin singlet.

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4:30PM D30.00009 Conductance enhancement of carbon nanotubes through metallization.
CATERINA SOLDANO, LI CHEN, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, SWASTIK KAR, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, SAIKAT TALAPATRA, Department of Physics, University of Southern Illinois at Carbondale, ROBERT VAJTAI, Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, SAROJ NAYAK, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, PULICKEL A. JAYAN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute — A novel method for building high-conductance device using carbon nanotubes is presented. The process involves a systematic, repeatable and controllable enhancement of the conductance using a rapid high-voltage cycling conducted in vacuum; this process leads to orders of magnitude drop in the two-terminal resistance. Electron microscopy analysis indicates that the high-bias cycling of nanotubes causes sufficient Joule heating for the platinum to migrate from the contact regions and decorate the outer surface of the nanotubes, giving rise to enhanced metallization. Pre- and post-metallization characterization is presented. It is believed that the conductance enhancement is due to a combination of a decrease in disorder density in the tube and an increase in the number of available channels for conductance. Those outcomes are investigated in the light of recently predicted theoretical models.

4:42PM D30.00010 Carbon nanotubes as tunable Luttinger liquids.
WADE DEGOTTIARDI, University of Illinois Urbana-Champaign, TZU-CHIEH WEI, Institute for Quantum Computing, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We investigate the properties of single-walled carbon nanotubes in transverse electric and magnetic fields. We find via band structure calculations that these fields can break particle-hole symmetry as well as that of the two Dirac points. Additionally, the speed of the left and right movers is generally different in the presence of both electric and magnetic fields. We consider the effect of these fields on Coulomb interactions within the tube and show that they can be used to tune the interaction parameter K associated with the Luttinger liquid properties of the tube. Finally, we discuss finite size effects and Coulomb blockade physics for holes. We further show that SO coupling determines the filling order in the many-electron ground states, in a way different than that expected from electron-electron interactions. At low magnetic fields we find that the two-electron ground state is neither a spin-triplet nor a spin-singlet, but a Slater determinant with wave functions that are predominantly spin singlet.

5:06PM D30.00012 Modeling Nanotube Networks For Semiconductor Channels and Sensors.
MEG NOAH, YOUNG-KYUN KWON, Nanomanufacturing Center of Excellence and Center for High-rate Nanomanufacturing, University of Massachusetts, LOWELL — We present a model to characterize ensembles of NT networks using properties of individual from measurement and from ab initio computations, and including changes in the presence of gases like NH$_3$, pressure, or external fields. From these, we simulate networks for user-specified channel shape, size and inhomogeneous NT mixtures. For example, the ensemble IV characteristics of 2 by 2 micron network can readily be compared to ensembles of 20 by 20 micron networks or 50 by 50 micron networks with 1 micron width for a wide variety of nanotubes characterized by independent length distributions for each chirality and then compared subjected to different environmental conditions. Validation with experimental data resulting from inhomogeneous NT mixtures is presented. Our goal is to optimize nanomanufacturing parameters like channel size for a user-defined application be it gas sensor, pressure actuator, or semiconductor answering questions like: “What is the statistical conductivity enhancement in the presence of NO$_2$?” “What radii yield the most semiconducting for 1 micron SWNT?” and “How does conductivity change as a function of gas density?” We focus on the fundamental understanding of nanocomposites.

5:18PM D30.00013 The Control of Electron Transport Related Defects in In situ Fabricated Single Wall Carbon Nanotube Devices.
ZHIXIAN ZHOU, Department of Physics and Astronomy, Wayne State University, ALASKA SUBEDI, GYULA ERES, RONGYING JIN, DAVID MANDRUS, Materials Science and Technology Division, Oak Ridge National Laboratory — Metallic single wall carbon nanotube (SWNT) devices were characterized using low temperature transport measurements to study how the growth conditions affect defect formation in carbon nanotubes. Suspended carbon nanotube devices were grown in situ by a molecular beam growth method on a pair of catalyst islands located on opposing Au electrodes fabricated by electron beam lithography. We present experimental evidence that transport related defect formation in carbon nanotubes, in addition to the well known growth temperature dependence, is also affected by the nature and the composition of the carbon growth gases. [Zhou et al., Appl. Phys. Lett. 89, 133124 (2006)] We have also investigated how the transport related defects affect the performance of SWNT field-effect-transistors, revealing significantly different impacts of the defects on semiconducting SWNT devices with Schottky and Ohmic contacts. [Zhou et al., unpublished]
2:30PM D31.00001 First Principles Studies of Tapered Silicon Nanowires: Fundamental Insights and Practical Applications, ZHI GANG WU, BNNI, University of California at Berkeley and Molecular Foundry, Lawrence Berkeley National Laboratory — Nanowires (NWs) are often observed experimentally to be tapered rather than straight-edged, with diameters (d) shrinking by as much as 1 nm per 10 nm of vertical growth. Previous theoretical studies have examined the electronic properties of straight-edged nanowires (SNWs), although the effects of tapering on quantum confinement may be of both fundamental and practical importance. We have employed ab initio calculations to study the structural and electronic properties of tapered Si NWs. As one may expect, tapered nanowires (TNWs) possess axially-dependent electronic properties; their local energy gaps vary along the wire axis, with the largest gap occurring at the narrowest point of the wire. In contrast to SNWs, where confinement tends to shift valence bands more than conduction bands away from the bulk gap, the unoccupied states in TNWs are much more sensitive to d than the occupied states. In addition, tapering causes the band-edge states to be spatially separated along the wire axis, a consequence of the interplay between a strong variation in quantum confinement strength with diameter and the tapering-induced charge transfer. This property may be exploited in electronic and optical applications, for example, in photovoltaic devices where the separation of the valence and conduction band states could be used to transport excited charges during the thermalization process. In order to gain insight into TNW photovoltaic properties, we have also carried out calculations of the dipole matrix elements near the band edges as well as the role of metal contacts on TNW electronic properties. Finally, a combination of ab initio total energy calculations and classical molecular dynamics (MD) simulations are employed to suggest a new technique for bringing nanoscale objects together to form ordered, ultra high-aspect ratio nanowires. This work was supported in part by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

3:06PM D31.00002 Structure and electronic properties of silicon nanowires grown along the [110] direction: role of surface reconstruction, T. AKIYAMA, K. NAKAMURA, T. ITO, Dept. of Phys. Eng., Mie Univ., Japan — Silicon single-crystal nanowires (SiNWs) are attracting great interest for future nanoscale devices in recent years. So far, the [110] grown SiNWs with diameters below 4 nm have been successfully fabricated by various methods. Although the size dependence in electronic and optical properties for the [110] grown SiNWs terminated by H-atoms have been intensively studied, effects of surface reconstructions on the electronic structure have rarely examined. Here, we investigate the atomic and electronic structures of SiNWs along the [110] direction with (001) and (111) facets using first-principles pseudopotential method. The calculations for SiNWs whose diameters are ~4 nm demonstrate that the reconstructions on these facets are strongly dependent on H-chemical potential $\mu_H$: The SiNW consisting of monohydride (001) and H-terminated (111) facets is stabilized for high $\mu_H$ ($\geq$0.75 eV) while the pristine SiNW stabilized for low $\mu_H$ ($\leq$-0.82 eV). The reconstructions with partially hydrogenated facets appear for -0.82$<\mu_H<$0.75 eV. Peculiar features in the electronic structure are also found in partially hydrogenated SiNWs.

3:18PM D31.00003 Modeling of Polycrystalline and Wurtzite Si Nanowires with Symmetry-Adapted Objective Molecular Dynamics, TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota, DONG-BO ZHANG, Department of Chemical Engineering and Materials Science, University of Minnesota, MING HUA, Department of Mechanical Engineering, University of Minnesota — The stability and properties of the most promising ground state candidate Si nanowires with less than 10 nm in diameter is comparatively studied with molecular dynamics coupled with non-orthogonal tight-binding and classical potential models. The computationally-expensive tight-binding treatment becomes tractable due to the substantial simplification in the number of atoms introduced by the presented symmetry-adapted objective molecular dynamics scheme. It indicates that the achiral polycrystalline of five-fold symmetry and the wurtzite wires of three-fold symmetry are the most favorable quasi one-dimensional Si arrangements. Quantitative differences with the classical model description are noted over the whole diameter range. Using a Wulff energy decomposition approach it is revealed that these differences are caused by the inability of the classical potential to accurately describe the interaction of Si atoms on surfaces and strained morphologies.

3:30PM D31.00004 Ab initio calculations for the electronic properties of zinc-doped indium phosphide nanowires, MANUEL ALEMANY, Universidad de Santiago de Compostela, Spain, XIANGYANG HUANG, University of Minnesota, MURILLO L. TIAGO, University of Texas at Austin, L.I. GALLEGO, Universidad de Santiago de Compostela, Spain, JAMES R. CHELIKOWSKY, University of Texas at Austin — p-type indium phosphide nanowires are known to function as working devices when assembled with n-type nanowires, and thus are seen as very promising building blocks for highly integrated electronic devices within the semiconductor industry. In this work, we have characterized the impurity state responsible for current flow in zinc-doped indium phosphide nanowires through first-principles calculations based on a real-space implementation of density-functional theory and pseudopotentials. The binding energy of the acceptor state is predicted to range from the value of the acceptor state in the bulk to upper values of approximately 0.2 eV in the thinner nanowires as a result of the two-dimensional quantum confinement. Our results show that, in thin nanowires, quantum confinement can move the defect level deep into the energy gap.

3:42PM D31.00005 Molecular-Dynamics Simulations of Nanowire Growth, TOMORR HAXHIMALI, Northwestern University and University of California at Davis, DOREL BUTA, MARK ASTA, University of California at Davis, JEFFREY HOYT, McMaster University — This talk will present results of molecular dynamics simulations investigating the mechanisms of nanowire growth from a liquid. We investigate the model system of elemental Si, modeled with the classical Stillinger-Weber potential. The work aims to investigate the effect of nanowire size on the intrinsic growth mechanisms and the relations between solid-liquid interface velocity, growth direction and driving force. Results will be presented for nanowires with diameters ranging from 5-10 nm, and will be compared with simulations for bulk Si modeled with the same potential. The consequences of these findings for the mechanisms of nanowire growth from liquid catalysts by the vapor-liquid-solid mechanism will be discussed.
3:54PM D31.00006 First-principles study of the electronic and magnetic properties of Fe-Co nanowires\(^1\). DANGXIN WU, PING LIU, QIMING ZHANG, University of Texas at Arlington, RUQIAN WU, University of California, Irvine — Fe-Co nanowires provide a potential way to produce high-performance nanocomposite permanent magnets due to their high Curie temperature, large magnetization, and appreciable anisotropy. In this talk we present our recent results of first-principles investigation of this matter. The calculations use both PAW method and FLAPW method, based on density functional theory. The structures of Fe-Co nanowires were optimized by PAW method and then the electronic structure and magnetic properties such as saturation magnetization and anisotropy energies are studied by FLAPW method. The effects of size and composition of the nanowires on the magnetic properties are also studied and compared with those of bulk Fe-Co materials.

\(^1\)This work was supported in part by the U.S. DoD/MURI under the Grant No. N00014-05-1-0497

4:06PM D31.00007 Magnetic Co impurity in Gold Nanowires\(^1\). EDISON DA SILVA, Instituto de Física "Gleb Wataghin", UNICAMP, Brazil, RENATO PONTES, ANTONIO J.R. DA SILVA, ADALBERTO FAZZIO, Instituto de Física, USP, Brazil — Nanoscale electric contacts using suspended gold nanowires (NWs) have recently been made and were imaged by electron microscopy. Using tools derived from Density Functional Theory (DFT) we study the role of magnetic impurities in these NWs with the possibility of spintronic applications. Here we study structural and transport properties of a gold nanowire with one Co impurity as function of tension applied to the NW. Co added new features to the physics of this system. We present studies of structure and also electronic transport using the same DFT formalism [1] that show the effect of the spin anisotropy introduced by Co. In particular, we present results of two geometries, one where the Co atom is connected to two Au atoms of the lead and another where it is in the middle of the suspended neck, in a linear configuration. In the former case we observe an interference between the s and d channels, leading to a Fano-like structure in the transmittance, whereas in the latter configuration there is a decoupling between these two channels and the transmittance has a simple peak around the Co d-states, leading to a large spin polarized transport. [1] F. D. Novaes, A.J.R. da Silva, and A. Fazzio, Braz. J. Phys. 36 (3A): 799-807 (2006)

3:40PM D31.00008 Transport in Carbon Nanotube Junctions\(^1\). HOANG VTU, V.S. MISHRA, University of Texas at Austin — There is growing interest in the use of carbon nanotube thin films as transparent electrical conductors and thin-film transistors owing to their high optical transmittance, low sheet resistivity, and ease of fabrication. [1,2] A major contribution to the sheet resistivity originates at nanotube junctions, as electrical contact is typically poor between adjacent nanotubes. It is thus important to characterize carbon nanotube junctions in order to understand the conduction properties of nanotube thin films. To this end, we have performed ab initio density functional theory calculations to investigate the structural, electronic, and transport properties of carbon nanotube junctions as a function of nanotube chirality and contact geometry.

\(^1\)This work was supported in part by FAPESP and CNPq. CENAPAD-SP is acknowledged for computer time.

4:18PM D31.00008 Transport in Carbon Nanotube Junctions\(^1\). K.H. KHOO, JAMES R. CHELIKOWSKY, University of Texas at Austin — There is growing interest in the use of carbon nanotube thin films as transparent electrical conductors and thin-film transistors owing to their high optical transmittance, low sheet resistivity, and ease of fabrication. [1,2] A major contribution to the sheet resistivity originates at nanotube junctions, as electrical contact is typically poor between adjacent nanotubes. It is thus important to characterize carbon nanotube junctions in order to understand the conduction properties of nanotube thin films. To this end, we have performed ab initio density functional theory calculations to investigate the structural, electronic, and transport properties of carbon nanotube junctions as a function of nanotube chirality and contact geometry.

\(^1\)This work was supported in part by the National Science Foundation under DMR-0551195 and the Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.

4:30PM D31.00009 Schottky Barrier Heights in CNT-Metal Junctions from First-principles\(^1\). NICHOLAS SINGH-MILLER, NICOLA MARZARI, Massachusetts Institute of Technology — Fundamental understanding of the electronic properties at the junction between carbon nanotubes and metal electrodes is important for the development of CNT-based devices. Here, we use density functional theory (DFT) to probe the properties of the CNT-metal interface, paying particular attention to the Schottky barrier heights (SBH). We focus on the junction between a semiconducting (8,0)CNT and aluminum or palladium, chosen as paradigmatic examples of a simple metal and a transition metal, respectively. We obtain SBHs from the potential lineup, examining the effects of geometry at the interface and the functionalization of the CNT on the SBH.

\(^1\)This work was supported in part by the National Science Foundation under DMR-0551195 and the Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.

4:42PM D31.00010 Transport properties of transition-metal-encapsulated Si cages\(^1\). LINGZHU KONG, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas at Austin — We performed density functional pseudopotential calculations of the spin dependent transport through transition-metal-atom-encapsulated Si cages $\text{Si}_2\text{X}(X=\text{Mn}, \text{Fe} \text{and} \text{Co})$. The effect of the metal atom on conductance is studied. Mn and Fe doped systems show highly spin polarized transmission whereas the magnetization in Co doped system is quenched. It is found that electrons are transferred from Si atoms into the minority d orbitals of the metal atoms. The conductance decreases as these electrons become localized around the encapsulated atoms.

\(^1\)This work was supported in part by the National Science Foundation under DMR-0551195 and the Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.


5:06PM D31.00012 Ab initio non-equilibrium Green’s function study on the growth of metallic bridge in mixed conductor atomic switch\(^1\). TOMOFUMI TADA, ZHONGCHANG WANG, TINGKUN GU, SATOSHI WATANABE, Dept. of Materials Engineering, The Univ. of Tokyo, JST-CREST — A novel atomic switch [1] composed of a mixed conductor, $\text{Ag}_2\text{S}$ or $\text{Cu}_2\text{S}$, has attracted much attention. To investigate the electronic properties of the atomic switch, we have examined interface structure and electron transport of $\text{Ag}/\text{Ag}_2\text{S}/\text{Ag}$ and $\text{Cu}/\text{Cu}_2\text{S}/\text{Cu}$ using ab initio non-equilibrium Green’s function method. In $\text{Ag}/\text{Ag}_2\text{S}/\text{Ag}$, we found a spontaneous growth of a metallic bridge composed of an Ag atomic chain when a unidirectional stress is applied to Ag$_2$S [2]. On the contrary, a metallic bridge does not appear in Ag$_2$S and Cu$_2$S without stress. We also examined the influence of Ag/Cu addition on the structural and transport properties of Ag$_2$S and Cu$_2$S atomic switches, and found that the Ag/Cu addition leads to the metallization in the both systems. However, clear growth of the atomic bridge is confirmed only in $\text{Ag}/\text{Ag}_2\text{S}/\text{Ag}$. The metallic nature in $\text{Cu}/\text{Cu}_2\text{S}/\text{Cu}$ is related to the growth of electronic charge network at the Fermi level. [1] K. Terabe, et al., Nature 433, 47 (2005). 2) Z. Wang, T. Kadohira, T. Tada, S. Watanabe, Nano Letters 7, 2688 (2007).
Magnetic field, sharp peaks at zero applied field when a large enough negative d.c. current, I, is applied. The oscillations extend from 0.6 to 4 GHz. They disappear when a 2\textsuperscript{nd} power is applied.

Except for the direction of I, these observations seem to be consistent with the vortex dynamics reported by the NIST and Cornell groups. If time permits, we will present results on magnetic nanopillars where the Py(24) layer has been replaced by NiCr, which inverts the spin asymmetry.

5:18PM D31.00013 Ab initio transport properties of platinum chains calculated by taking into account spin-orbit effects, VICTOR GARCIA-SUAREZ, Lancaster University, DAVID ZSOLT MANRIQUE, Universidad de Oviedo, COLIN LAMBERT, Lancaster University, JAIME FERRER, Universidad de Oviedo — The transport properties of infinite and finite platinum chains are calculated by using a combination of Density Functional Theory and Non-Equilibrium Green’s Functions Formalism, as implemented in the Smeagol Code. We show that spin-orbit effects, which are included fully self-consistently in our calculations, are of paramount importance to determine accurately the electronic and transport characteristics of these systems. For infinite chains we find that under special circumstances which depend on the type of chain (linear or zigzag), length and spin orientation relative to the chain, the conductance can be totally suppressed, giving rise to large magnetoresistive ratios. In the case of finite chains between bulk electrodes the spin-orbit effect plays also a crucial role and gives results which agree better with experiments.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D32 GMAG DMP FIAP: Focus Session: Spin Transfer Torque I
Morial Convention Center 225

2:30PM D32.00001 Switching behavior of a Stoner-Wohlfarth particle subjected to spin-torque effect\textsuperscript{1}, HUY PHAM, Advanced Materials Research Institute, University of New Orleans, DORIN CIMPORU, AMRI, University of New Orleans, ALEXANDRU STANCU, “Al. I. Cuza” University, Faculty of Physics, Iasi 700506, Romania, LEONARD SPINU, AMRI, University of New Orleans — The concept of the “spin-transfer torque” proposed by Slonczewski and Berger offers a new way of controlling the magnetization reversal in ferromagnetic multilayer systems, which replaces the conventional method utilizing magnetic field. The novel technology is expected to reduce the switching time of magnetization as well as to increase the recording density of the magnetoresistive random access memories. In this paper the switching properties of a Stoner-Wohlfarth magnetic particle, subject to a continuous or short magnetic field pulses, and to a short current pulse are presented. The theoretical investigation of precessional motion is described by using phenomenological modified Landau-Lifschitz-Gilbert equation with a spin-transfer torque term included. The switching under the influence of spin transfer torque is discussed as a function of the applied field strength and direction, and also as a function of the length of the current pulse. The main goal is to determine the parameters of field pulse for that the fast and stable switching can be achieved.

\textsuperscript{1}Supported in part by NSF DMR-0747609

2:42PM D32.00002 Dynamical Coupling of Nanomagnets due to Spin Transfer\textsuperscript{1}, SERGEI URAZHDIN, West Virginia University, WENG-LEE LIM, NICHOLAS ANTHONY, ANDREW HIGGINS — Spin transfer devices typically incorporate a thick magnet polarizing the electric current, and a thin layer driven by spin torque. However, spin torque acting on both layers is significant in devices with comparable thickness of magnetic layers. Moreover, dynamics of one of the magnetic layers results in oscillations of the polarization of the current flowing through the other layer, which can lead to dynamical coupling between them. We discuss results of simulations and measurements, demonstrating several consequences of such dynamical coupling. First, the dynamics of both layers are always simultaneously excited by the current. Second, the critical current for the onset of magnetic dynamics is scaled by the ratio of the thicknesses of the magnetic layers, diverging when the two are the same. This behavior is caused by the coupled precession of two magnetic layers reducing the efficiency of spin transfer. Below the critical current, a hysteretic regime is found in which a dynamical state and a static parallel configurations are possible. This regime may explain the 1/f noise and broad precession peaks that are often observed in the spectra of current-induced excitations.

\textsuperscript{1}Partly supported by NSF DMR-0747609

2:54PM D32.00003 Magnetic propeller driven by spin transfer\textsuperscript{1}, WENG LEE LIM, NICHOLAS ANTHONY, ANDREW HIGGINS, SERGEI URAZHDIN, Department of Physics, West Virginia University, Morgantown WV 26506 — Spin-transfer devices usually contain two magnetic layers in which the thicker layer polarizes the electron current and the thinner layer experiences dynamics due to spin transfer. However, both magnetic layers can polarize current and experience simultaneous dynamics when the thickness of magnetic layers is similar (symmetric nanopillars). We investigated current-driven magnetization switching in symmetric nanopillars with structure NiFe20/Pt= Py(4nm)/Cu(3.5nm)/Py(4nm). Time-resolved measurements of resistance for both directions of current and magnetic field showed reversible switching of magnetization between parallel (P) and anti-parallel (AP) states with unusual dependence on the current. We observed that the dwell times displayed two different dependences on the current I for different values of applied field H. At large H, the dwell time in the P state t\textsubscript{P} decreases with increasing I while the dwell time in the AP state t\textsubscript{AP} increases, similarly to asymmetric devices. However, at small H, both t\textsubscript{P} and t\textsubscript{AP} decrease with increasing I. We explain this unusual behavior by a thermal activation model involving four-cycle sequential reversal of two magnetic layers.

\textsuperscript{1}Partly supported by NSF DMR-0747609.

3:06PM D32.00004 Coherence of spin-torque microwave oscillators, ANDREI SLAVIN, Oakland University — Recently discovered effect of microwave generation in current-driven magnetic nano-structures caused by the spin-transfer torque opens a possibility for the development of a new type of tunable microwave auto-oscillators. The spin-torque oscillators (STO) are strongly nonlinear as their frequency \(\omega(P)\) and total (positive plus negative) damping \(\Gamma(P)\) are dependent on the oscillation power \(P\). We developed a theory of the generation linewidth of a nonlinear auto-oscillator, and showed that the nonlinear frequency shift (characterized by the coefficient \(N = d\omega/dP\)) leads to an effective increase of the phase noise. In a strongly supercritical regime, when the oscillation energy \(E(P)\) is much larger than the thermal energy \(k_BT\), the generation linewidth of a STO can be written as \(\Delta\omega = \Delta\omega_0[1 + (N/T_{\text{eff}})^2]\), where \(\Delta\omega_0 = \Gamma(0)/(k_BT/E(P))\) is the oscillator linewidth without account for the nonlinear frequency shift and \(T_{\text{eff}} = dT/dP\) is the effective nonlinear damping of the oscillator. Our theory explains the following features of the STO linewidth observed in experiment: (i) general linewidth narrowing with the increases in the bias current \(I\) and the oscillation energy \(E(P)\), (ii) presence of a minimum in the linewidth dependence on the orientation of the external bias magnetic field; (iii) linear dependence of the linewidth on the absolute temperature. Our theory also demonstrates that in the array of \(n\) phase-locked STO the generation linewidth decreases linearly with the increase on the number of oscillators \(n\), while the generated power \(P\) increases as \(n^2\).

3:42PM D32.00005 Magnetization excitations in magnetic nanopillars induced by a d.c. spin-polarized current\textsuperscript{1}, NIKOLETA THEODOROPOULOU, AMIT SHARMA, WILLIAM PRATT JR., JACK BASS, Dept. of Physics and Astronomy, Michigan State University — We have measured spin-transfer-torque driven magnetization dynamics at 293K in Py(24nm)/Cu(10nm)/Py(6) magnetic nanopillars, with the top Py(6) magnetic layer and part of the Cu layer shaped into a 140x70 nm\textsuperscript{2} ellipse, and the rest left extended. Among the more interesting results are sharp peaks at zero applied field when a large enough negative d.c. current, I, is applied. The oscillations extend from 0.6 to 4 GHz. They disappear when a magnetic field, \(B_{\text{eff}}\), larger than 10 mT is applied in the plane of the layers, but persist up to 0.2 T when \(B_{\text{eff}}\) is applied perpendicular to this plane. The peaks persist up to 5-9 times the switching current and appear to be current-hysteric. At \(B_{\text{eff}} = 0\), the frequency of the oscillations increases with \(I\) (\(\sim 40\text{MHz}/\text{mA}\)). Except for the direction of I, these observations seem to be consistent with the vortex dynamics reported by the NIST and Cornell groups. If time permits, we will present results on magnetic nanopillars where the Py(24) layer has been replaced by NiCr, which inverts the spin asymmetry.

\textsuperscript{1}Supported in part by NSF grant DMR-05-01013.
3:54PM D32.0006 Resonant Spin-Transfer-Driven Switching of Magnetic Spin Valves Assisted by Microwave Current Pulses, YONG-TAO CUI, JACK C. SANKEY, CHEN WANG, KIRAN V. THADANI, ZHI-PAN LI, ROBERT A. BUHRMAN, DANIEL C. RALPH, Cornell University — Spin transfer torque from an electrical current can reverse the magnetization in a nanomagnet. We show experimentally that applying a microwave-frequency current pulse in addition to a DC pulse can improve switching characteristics at low temperature by exciting a nanomagnet resonantly at its precession frequency. We study spin valve nanopillars with the structure IrMn(8 nm)/permalloy(4 nm)/Cu(8 nm)/permalloy(4 nm) where exchange bias causes an initial offset angle of ∼45 degrees between the permalloy magnetizations. We apply nanosecond-scale microwave-frequency current pulses prior to completing the switching with a DC current pulse. We find that the probability of successful switching has a resonant dependence on frequency, and it also depends on the phase of the microwaves at the moment when the DC pulse is applied. With a microwave pulse, the DC pulse length required for switching is shorter and has a narrower distribution compared to switching driven by a DC pulse alone.

4:06PM D32.00007 Phenomenological model for size-dependent switching behavior in spin transfer torque devices, VENKATESH CHEMBROLU, Department of Applied Physics, Stanford University, Stanford, California 94305, USA, YVES ACREMANN, PULSE Centre, Stanford Linear Accelerator Centre, Menlo Park, California 94025, USA, JOHN PAUL STRACHAN, XIAOWEI YU, Department of Applied Physics, Stanford University, Stanford, California 94305, USA, ASHWIN TULAPURKAR, Stanford Synchrotron Radiation Laboratory, Menlo Park, California, 94025, USA, JORDAN KATINE, MATHEW CAREY, Hitachi Global Storage Technologies San Jose Research Center, San Jose, California 95120, USA, TOLEK TYLISZCZAK, Advanced Light Source, Berkeley, California, 94720, JOACHIM STOHR, Stanford Synchrotron Radiation Laboratory, Menlo Park, California 94025, USA — Recent results based on time resolved x-ray imaging of magnetization dynamics in nano-magnetic devices have shown size dependent trends in the switching behavior. Samples with a lateral dimension of 100x180nm show a vortex-driven switching mechanism, whereas smaller samples with a lateral dimension of 110x150nm do not switch by a vortex. Further studies have shown that when a non-zero angle in introduced between the fixed and the free layers, vortex-driven switching becomes manifest in samples with smaller dimensions also. Here, we would like to present a phenomenological model based on linearized LLG equations to explain the various regimes of observed switching behaviors.

4:18PM D32.00008 Linewidths of Spin-Torque-Driven Nanomagnetic Oscillators as a Function of Field Angle and Temperature, KIRAN V. THADANI, Z.-P. LI, O. OZATAY, J.C. SANKEY, I.N. KRIVOROTOV, Y.-T. CUI, R.A. BUHRMAN, D.C. RALPH, Cornell University, G. FINOCCHIO, U. of Messina (Italy) — In a magnetic multilayer device, spin-transfer torque from a direct current can excite steady-state magnetic oscillations. We observe that the linewidths of the oscillations decrease dramatically as an applied magnetic field is rotated away from the magnetic easy axis towards the in-plane hard axis. Micromagnetic simulations show that the spatial coherence of the oscillations improves greatly as the field is rotated, and their amplitude tends to zero, making them less susceptible to thermal fluctuations. We report the temperature dependence of the linewidths for the field directions giving the minimum linewidths. It has been suggested previously that the linewidths are dominated by fluctuations of the precession angle of the nonlinear oscillator [1,2]. We analyze the mechanisms governing our linewidths by comparing them to micromagnetic modeling. [1] J. C. Sankey et al., Phys. Rev. B 72, 224427 (2005). [2] J.-V. Kim et al., cond-mat/0703317.

4:30PM D32.00009 Enhancement in spin-torque efficiency by nonuniform spin current generated within a tapered nanopillar spin valve, P.M. BRAGANCA, O. OZATAY, A.G.F. GARCIA, O.J. LEE, D.C. RALPH, R.A. BUHRMAN, Cornell University — When modeling spin torque related phenomena, it is generally assumed that the polarization of the incident current is spatially uniform and invariant in time across the surface of the free layer nanomagnet. This is not necessarily the case for a relatively thick, low saturation magnetization free layer nanomagnet. Here, we discuss the results of spin-torque micromagnetic simulations, confirmed by both dc and short-pulse switching measurements of nanopillar spin valve structures, which reveal that the use of this type of reference layer can result in non-uniform polarization of the current that impinges onto the free layer. This effect can enhance magnetic reversal in the nanosecond-switching regime over the case of a fixed and uniformly magnetized reference layer, substantially reducing the current amplitude required for magnetic reversal with a given ns pulse-width. We will discuss these results, which differ substantially from descriptions provided using macrospin approximations, and describe a nanopillar-torque device configuration that simulations and experiments indicate could be quite effective in reducing the spin torque switching current for MRAM applications.

4:42PM D32.00010 Theory of Ferromagnetic Resonance in Perpendicularly Magnetized Nanodiscs: Excitation by Injected AC Current1, RODRIGO ARIAS, Departamento de Física, FCFM, Universidad de Chile, DOUGLAS MILLS, Department of Physics and Astronomy, UC Irvine — Recent experiments explore the ferromagnetic resonance (FR) response of nanodiscs incorporated into nanopillars, where a DC spin torque current has a small AC component superimposed. For such a circular perpendicularly magnetized disc, we develop the theory of the FR response via AC current. Earlier we discussed the vortex state induced by the DC Oersted field in such a sample, and the nature of the spin waves in the presence of the vortex2. The present study explores the linear response of the disc, when a small AC current is superimposed on the DC current. A Green’s function approach allows us to describe the linear response of the system. We argue that the AC component of the Oersted field is responsible for spin wave excitation; the modes excited thus differ from those observed in ferromagnetic resonance studies via microwaves. We shall present calculations which explore the spectrum and eigenvectors of modes excited by modulation of the DC current, their width as a function of DC current, and their intensity. 2R. E. Arias and D. L. Mills, Phys. Rev. B75, 214404 (2007).

4:54PM D32.00011 Quantum transport in Spin Torque Transfer Devices, SAYEEF SALAHUDDIN, DEEPANJAN DATTA, PRABHAKAR SRIVASTAVA, SUPRIYO DATTA, Purdue University — We present a simulation of a tunneling based Spin Torque Transfer (STT) devices using the Non Equilibrium Greens Function (NEGF) formalism in the ballistic regime. Our method is based on effective mass treatment of the magnetic contacts and tunneling oxide, including the effect of transverse modes in the transverse direction. We show that it is possible to achieve a quantitative agreement with experiments for both the tunneling magneto resistance (TMR) and the amplitude of the switching current with the same set of device parameters [1]. We shall talk about some implications of these results in the context of improving the device performance. We shall also briefly discuss how the nature of the torque may change if there is spin flip scattering. [1] S.Salahuddin, Deepanjan Datta, Prabhakar Srivastava and Supriyo Datta, proceedings of International Electron Devices Meeting (IEDM), 2007.

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1DLM acknowledges support from the U. S. Army from Contract CS00128; R. E. A. from FONDECYT, No. 1061106 (Chile).
5:06PM D32.00012 Spin Pumping of Current in Non-Uniform Conducting Magnets1, WAYNE SASLOW, Texas A&M University — Using irreversible thermodynamics we show that current-induced spin transfer torque within a magnetic domain implies spin pumping of current within that domain. This has experimental implications for samples both with conducting leads and that are electrically isolated. These results are obtained by deriving the dynamical equations for two models of non-uniform conducting magnets: (1) a generic conducting magnet, with net conduction electron density $n$ and net magnetization $M$; and (2) a two-band magnet, with up and down spins each providing conduction and magnetism. For both models, in regions where the equilibrium magnetization is non-uniform, voltage gradients can drive adiabatic and non-adiabatic bulk spin torques. Oseen relations then ensure that magnetic torques likewise drive adiabatic and non-adiabatic currents – what we call bulk spin pumping. For a given amount of adiabatic and non-adiabatic spin torque, the two models yield similar but distinct results for the bulk spin pumping, thus distinguishing the two models. As for recent spin-Berry phase work, we find that within a domain wall the ratio of the effective emf to the magnetic field is approximately given by $\mu(2\mu B/e)$, where $\mu$ is the spin polarization. The adiabatic spin torque and spin pumping terms are shown to be dissipative.

1Supported by Department of Energy grant DE-FG02-06ER46278.

5:18PM D32.00013 First principles calculation of the spin transfer torques, KE XIA, YUAN XU, SHUAI WANG, Institute of Physics, Beijing — A first principles method was developed to calculate the spin transfer torques in the noncollinear magnetized system. We found that the behavior of spin torques in a spin valve depends on the materials(Co, Ni and NiFe20), taken into account). The formalism is also applied to the antiferromagnetic domain wall. It is found that the spin torques could be exerted over a long range in the anti-ferromagnetic materials and move the domain wall away, which can be detected by measuring the resistance of an antiferromagnetic point contact.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D33 DMP GMAG FIAP: Focus Session: Spin Dependent Phenomena in Semiconductors: III Morial Convention Center 224

2:30PM D33.00001 Theory of Current-Induced Domain Wall Creep in (Ga,Mn)As, JUN’ICHI IEDA, Institute for Materials Research, Tohoku University — A magnetic domain wall (DW) can interact with electrical current and as a result its displacement is induced by the application of the current, showing the possible electrical control of the magnetization direction. Thus electrical current in this non-uniform spin texture is now drawing much attention from the technological point of view, in addition to the longstanding interests from the fundamental physics points of view. Recently, systematic experimental data of the dependence of DW velocity spanning five decades on current density have been obtained in a microstructure made from a ferromagnetic semiconductor (Ga,Mn)As, providing deep insight to outstanding physics of DW dynamics. The quantitative analyses showed that the current-driven motion in (Ga,Mn)As can be explained by spin-transfer mechanism under currents beyond a threshold value. The linear mobility tempts ones to expect that there is always an equivalent magnetic field which has the same effect upon DWs as the current does. Here we make a detailed comparison between these two sources of drive but in the subthreshold, “creep,” regime, where the velocity obeys an Arrhenius scaling law. The observed scaling law for the two drives is incompatible different from each other, i.e., the effect of a driving current and field are not equivalent. We offer theory which explains the important features of experiment. When described by an Arrhenius law it is found that the barriers diverge as the drive approaches zero, manifesting the system is in a “glassy” state. While the field driven case is compatible with the random field universality class, the case of current induced creep is not to fit any known such class. The work reported is the result of collaborations with M. Yamanouchi, F. Matsukura, S. E. Barnes, S. Maekawa, and H. Ohno. [Ref. Science 317, 1726-1729 (2007)].

3:06PM D33.00002 Analyzing the influence of magnetic domain walls on longitudinal and transverse magnetoresistance in tensile strained (Ga,Mn)As, GANG XIANG, Dept. of Physics, Ohio State University, NITIN SAMARTH, Dept. of Physics, Pennsylvania State University — We present a theoretical analysis of magnetoresistance in (Ga,Mn)As epilayers with perpendicular magnetic anisotropy [Phys. Rev. B 76, 054440 (2007)]. The model reproduces the field-antisymmetric anomalies observed in experimental measurements [Phys. Rev. B 71, 241307(R) (2005)] of the longitudinal magnetoresistance in the planar geometry (magnetic field in the epilayer plane and parallel to the current density), as well as the unusual shape of the accompanying transverse magnetoresistance. As in the case of metallic ferromagnets with perpendicular anisotropy [Phys. Rev. Lett. 94, 017203 (2005)], the magnetoresistance characteristics are attributed to circulating currents created by the presence of magnetic domain walls.

3:18PM D33.00003 Manipulation of Magnetic Domain Walls in Patterned (Ga,Mn)As Devices, ANDREW BALK, Dept. of Physics, The Pennsylvania State University, MENG ZHU, Dept. of Physics, Penn State University, NITIN SAMARTH, Dept. of Physics, The Pennsylvania State University, DAVID AWSCHALOM, Dept. of Physics, University of California, Santa Barbara — Ferromagnetic semiconductors such as (Ga,Mn)As provide new opportunities for electrical manipulation of magnetic domain walls in a different regime of parameter space compared with ferromagnetic metals [Chiba et al, PRL 96, 096602 (2006)]. Here, we discuss different approaches to pinning and controlling magnetic domain walls in laterally patterned (Ga,Mn)As microdevices with perpendicular magnetic anisotropy. The pinning/postinning of domain walls is monitored using measurements of the magnetoresistance, the anomalous Hall effect and high speed Kerr microscopy. The domain wall pinning potential is engineered using a variety of schemes, including lateral shape engineering and lithographically integrated micromagnets. We find that even simple schemes (such as lateral notches) can significantly enhance domain wall pinning in relatively large (micron scale) devices. Supported by ONR MURI.

3:30PM D33.00004 Spin valve effect in self-exchange biased ferromagnetic metal/semiconductor heterostructures1, MENG ZHU, MARK WILSON, BEN-LI SHEU, PARTHA MITRA, PETER SCHIFFER, NITIN SAMARTH, Pennsylvania State University — The systematic engineering of exchange biased ferromagnetic semiconductor spin valve devices is important for developing proof-of-concept semiconductor spintronics devices (such as spin torque oscillators). Here, we report magnetization and current-perpendicular-to-the-plane (CPP) magnetoresistance measurements in hybrid ferromagnetic metal/semiconductor heterostructures built from MnAs and (Ga,Mn)As. [Appl. Phys. Lett. 91, 192503 (2007)]. We observe an exchange biased CPP spin valve effect in MnAs/(Ga,Mn)As bilayers, and discuss the dependence of the exchange field and the spin valve effect on (Ga,Mn)As layer thickness. We also demonstrate the CPP spin valve effect and exchange biasing in MnAs/p-GaAs/ (Ga,Mn)As trilayers, and discuss the dependence of both phenomena on the doping and thickness of the non-magnetic spacer layer.

1Work supported by the ONR MURI program.
The influence of the Doping Profile on Spin Transport in Fe/GaAs Schottky Tunnel Barrier Heterostructures, Q. Hu, E.S. Garlid, K.S.M. Reddy, J. Zhang, T. Kondo, P.A. Crowell, C.J. Palmström, University of Minnesota—A strong non-monotonic dependence of the spin polarization on the bias across the injector has been observed in recent studies of spin transport in Fe/GaAs heterostructures. We have conducted a study of spin transport in non-local Fe/GaAs spin valves in which the doping profile of the Schottky barrier has been systematically modified. The samples were Fe/n+/n-GaAs heterostructures in which the thickness d of the n+ layer (n+ fixed at 5 × 10¹⁸ cm⁻³) was varied from 5 nm to 50 nm while n ≈ 5 × 10¹⁶ cm⁻³ in the 2.5 μm thick channel. We performed non-local spin valve measurements at 15 K for unannealed samples and after annealing at 200°C and 250°C. For d less than 10 nm, no spin accumulation is observed under either forward or reverse bias. For d ≥ 15 nm, spin accumulation is observed under forward bias only. Spin accumulation is observed for both bias polarities at larger thicknesses, with an optimal d ≈ 20-25 nm. Although this overall trend with d is observed in both unannealed and annealed samples, the sign and magnitude of the non-local signal can change upon annealing. These results suggest that spin accumulation is sensitive to both the tunnel barrier profile and interfacial conditions. This work was supported by ONR and the NSF MRSEC, IGERT, and NNNI programs.

Single domain switching by spin-polarized current in GaMnAs nanodevice, A. Chernyshov, M. Overby, L.P. Röhrinson. Department of Physics, Purdue University, West Lafayette, IN 47907, J.K. Furdyna, X. Liu. Department of Physics, University of Notre Dame, Notre Dame, IN 46556—Dilute magnetic semiconductors (DMS) have a potential to bring electrostatic control into magnetic domain and bridge the gap in control efficiency between conventional ferromagnetic materials and semiconductors. A significant progress has been demonstrated in current-induced magnetization reversal, where DMS materials show a few orders of magnitude current reduction compared to the conventional ferromagnets. In this work we demonstrate and investigate in-plane single domain magnetization rotation and reversal in GaMnAs nanodevices by spin-polarized dc electric field. Single domain is defined lithographically, which eliminates ambiguity associated with previously investigated multi-domain switching. The magnetization orientation can be controllably switched between two 100 and 010 easy axes or reversed. Current alone is not sufficient to switch the magnetization and have been aided by small in-plane magnetic field (~10mT). We observe linear dependence of critical currents with respect to magnetic field and analyze it in terms of current induced torque on the domain walls. The critical current densities are of the same order as for out-of-plane magnetization switching reported by Ohno, et al.

Magnetoresistance Enhancement through a Resonant Tunneling Diode based in the GaMnAs/AlGaAs Materials System, Edward Likovich, Kasey Russell, Wei Yi, Venkatesh Narayanamurti, Harvard University, Keh-Chiang Kuo, Meng Zhu, Nitin Samarth, Penn State University—A resonant tunneling diode was fabricated with ferromagnetic GaMnAs emitter and quantum well regions and a nonmagnetic p-GaAs collector. Negative differential resistance (NDR) associated with resonant tunneling of holes was observed at 4K, which is below the Curie temperature for GaMnAs. If the device bias is held constant and the magnetic field is swept, our device exhibits either positive or negative tunneling magnetoresistance (TMR) up to 30%, depending on device bias. Current-voltage sweeps reveal the source of the magnetoresistance as a shift in the NDR features to higher bias when the magnetizations of the GaMnAs films become antiparallel. We attribute this bias shift to an increase in tunneling conductivity from the emitter to quantum well for antiparallel GaMnAs magnetization alignment.

Dissipationless transport properties and Mott relation in Ga₁₋ₓMnₓAs, Yong Pu, Jiyong Sheng, Dept. of Physics, UC-Riverside, Daichi Chiba, Erato, JST, Rie, Tohoku University, Fumihiro Matsukura, Hideo Ohno, Rie, Tohoku University, Erato, JST—We have found an anomalously large Nernst effect (ANE) accompanying the anomalous Hall effect (AHE) in a series of Ga₁₋ₓMnₓAs (x=0.04-0.07) ferromagnetic semiconductor samples with perpendicular anisotropy. Without applying a magnetic field, none-zero ANE and AHE are observed, and both effects are very well scaled with the sample magnetization. We have developed a method, which does not depend on the accuracy of magnetization measurement, to study the anomalous transport effects. By measuring AHE and ANE under zero magnetic field and over a wide range of temperatures, we have demonstrated the dissipationless origin of the anomalous electrical and thermolectric transport properties in these samples. Furthermore, we have successfully verified the Mott relation for the off-diagonal transport coefficients in the regime of dissipationless transport that may not depend on scattering.

Localization effects in ferromagnetic Ga₁₋ₓMnₓSb random alloys, M. Eginligil, G. B. Kim, H. Luo, B. D. Mccombe, Dept. of Physics, University at Buffalo, Sunny Y. S. Yoon, J. P. Bird, Dept. of Electrical Engineering, University at Buffalo, SUNY—We have investigated temperature and magnetic field dependence of resistance (Rₓₓ) in MBE-grown ferromagnetic Ga₁₋ₓMnₓSb films in which ferromagnetism is mediated by holes. Samples with higher carrier densities (6.7 × 10¹⁷ cm⁻³ - 3.0 × 10²⁰ cm⁻³) with Curie temperatures, Tc, of 13 K and 24 K respectively show metal-like behavior in the temperature dependence of Rₓₓ. These samples exhibit small positive magnetoresistance (MR) up to 0.5 Ω between 1.6 K and 20 K, followed by negative MR up to 10 and 11 Ω (at 2.4 K), respectively. Samples with lower carrier densities (2.9 × 10¹⁷ cm⁻³ - 3.9 × 10¹⁶ cm⁻³), with Tc’s of 13 K and 24 K, respectively show “weak” thermally activated behavior and negative MR between 1.6 K and 50K (but no positive MR at low fields). The latter samples exhibit low-field positive MR between 35 mK and ~ 400 mK, followed by negative MR up to 8 T. Rₓₓ increases with decreasing temperature for both zero field, and the magnitude of the change increases with applied magnetic field. These results will be discussed in terms of localization behavior in this system. [1] Eginligil et al., in press PhysicaE (2007)

Huge tunneling magnetoresistance (>18300%) in semiconductor based magnetic tunnel junctions with zinc-blende MnAs nanoparticles, Pham Nam Hai, Byungho Yu, Dept. of Electronic Eng., The Univ. of Tokyo, Shindou Ohya, Masaoaki Tanaka, Dept. of Electronic Eng., The Univ. of Tokyo; JST—Zinc-blende (ZB) MnAs nanocrystalline is a new prospective material for semiconductor spintronics, since it is expected to be half-metallic. However, there is no report on the magneto-transport characteristics of ZB MnAs nanoparticle system. In this paper, we report on the huge tunneling magnetoresistance (TMR) effect in MBE-grown magnetic tunnel junctions (MTJs), whose structure is (from the top to the bottom) hexagonal MnAs film (20 nm)/GaAs (1 nm)/AlAs (2.1 nm)/GaAs:MnAs (10 nm), revealing the half-metallicity of ZB MnAs nanocrystallite. Here, the GaAs:MnAs layer contains ZB MnAs nanoparticles embedded in a GaAs matrix. The tunnel resistance decreases sharply with increasing the magnetic field, resulting in a huge TMR ratio = (R₉₀₀₋₅₅₀ / R₅₅₀). The TMR ratio decreases quickly with increasing the bias voltage and temperature, but survives up to 100 K. Such a huge TMR effect can be explained by an unique combination of Coulomb Blockade effect and large Zeeman splitting in half-metallic ZB MnAs nanoparticles. A magnetic-field dependent electromotive force emerged from those MTJs was also observed.
4:54PM D33.00011 Ultrafast Photoinduced Demagnetization in (III,Mn)V Ferromagnetic Semiconductors1, LUKASZ CYWINISKI, Condensed Matter Theory Center, University of Maryland — Ultrafast light-induced demagnetization, in which photoexcitation leads to a decay of magnetization in less than a picosecond, has been recently observed in (III,Mn)V materials [1]. To explain these measurements, we have proposed a theory of ultrafast magnetization dynamics within the sp-d model [2]. We have calculated the spin-flip scattering between the localized spins and the carriers strongly excited by the laser pulse. In this process the energy is pumped into the localized spin system, while the angular momentum is transferred to the carriers, leading to their dynamical spin polarization. For significant ultrafast demagnetization, this polarization has to be efficiently relaxed by spin-orbit assisted scattering of carriers - otherwise a “spin bottleneck” can occur, in which the carriers’ spin relaxation quickly becomes large enough to suppress further spin-flip scattering. Because of that, and also due to their larger exchange coupling to Mn spins, the holes (having a very short spin relaxation time) are much more important than photoelectrons for demagnetization. Since the spin-flip transition rate is proportional to the carrier temperature, the time-scale for this two-step process of demagnetization is given by the energy relaxation time of very hot holes. I will discuss in detail the application of this theory to (III,Mn)V semiconductors taking into account their valence band structure, and the fact that their optical properties are strongly affected by disorder inherent to these materials.


1 This research was done at University of California, San Diego and it was supported by NSF.

Monday, March 10, 2008 2:30PM - 5:18PM — Session D35 FIAP: Focus Session: Negative Index Materials II Morial Convention Center 227

2:30PM D35.00001 Negative Index Metamaterials for Superlenses Based on Metal-Dielectric Nanocomposites1, LATIKA MENON, WENTAO LU, ADAM FRIEDMAN, STEVEN BENNETT, DONALD HEIMAN, SRINIVAS SRIDHAR, Northeastern University — Negative index metamaterials are demonstrated based on metal-dielectric nanocomposites. The nanocomposites are prepared using a versatile bottom-up nanofabrication approach involving the incorporation of vertically aligned metal nanowires such as Au and Ag inside dielectric aluminum oxide nanotemplates. Aluminum oxide nanotemplates with specific pore dimensions are fabricated by means of electrochemical anodization. Following this, Au/Ag nanowires with specific wire dimensions are electrodeposited inside the pores. Optical absorbance measurements show resonance peaks corresponding to transverse and longitudinal surface plasmon modes. Peak position and intensity are found to be strongly dependent on nanocomposite dimensions, filling factor (ratio of the volume of metal versus the volume of dielectric) and angle of incidence with respect to the wire axis. A quantitative model based on effective medium theory in excellent agreement with experimental data, and points to specific composite configurations and wavelength regimes where such structures can have applications as negative refraction media for superlens imaging.

1 AFRL Hanscom,FA8718-06-C-0045, PHY-0457002, DMR-0305360

2:42PM D35.00002 Anisotropic nanostructured metamaterials for broadband all-angle negative refraction and flat lens imaging1, WENTAO LU, SRINIVAS SRIDHAR, Department of Physics and Electronic Materials Research Institute, Northeastern University, Boston, Massachusetts 02115, USA — We show that a metamaterial consisting of aligned metallic nanowires in a dielectric matrix has strongly anisotropic optical properties. For filling ratio f < 1/2, the composite medium shows two surface plasmon resonances (SPRs): the transverse and longitudinal SPR with wavelengths \( \lambda_t < \lambda_l \). For \( \lambda_t > \lambda_l \), the longitudinal SPR, the material exhibits \( \text{Re} \varepsilon \perp < 0 \), \( \text{Re} \varepsilon_\parallel > 0 \), relative to the nanowires axis, enabling the achievement of broadband all-angle negative refraction and flat lens (superlens) imaging systems. High performance systems made with Au, Ag or Al nanowires in nanoporous templates are designed and predicted to work from the infrared up to ultraviolet frequencies.

1 This work was supported by the Air Force Research Laboratories, Hanscom (Contract # FA8718-06-C-0045) and the National Science Foundation (contract # PHY-0457002).

2:54PM D35.00003 Achieving sub-diffraction imaging through bound surface states in negative-refracting photonic crystals at the near-infrared, ROHIT CHATTERJEE, Optical Nanostructures Laboratory, Solid-State Science and Mechanical Engineering, Columbia University, New York, NICOLAE PANOIU, Department of Electronic and Electrical Engineering, University College London, London, KAI LIU, ZACHARY DIOS, Optical Nanostructures Laboratory, Solid-State Science and Mechanical Engineering, Columbia University, New York, MING BIN YU, MY THE DOAN, The Institute of Microelectronics, Singapore, LAURA KAUFMAN, Department of Chemistry, Columbia University, New York, RICHARD OSGOOD, Department of Applied Physics and Applied Mathematics, Columbia University, New York, CHEE WEN WONG, Optical Nanostructures Laboratory, Solid-State Science and Mechanical Engineering, Columbia University, New York — We report the observation of imaging beyond the diffraction limit due to bound surface states in negative refraction photonic crystals. We achieve an effective negative index figure-of-merit \([\text{Re}(\varepsilon_\parallel)/\text{Im}(\varepsilon_\parallel)]\) of at least 380, \( \sim 125 \times \) improvement over recent efforts in the near-infrared, with a 0.4 THz bandwidth. Supported by numerical and theoretical analyses, the observed near-field resolution is 0.47\( \lambda \), clearly smaller than the diffraction limit of 0.61\( \lambda \). Importantly, we show this sub-diffraction imaging is due to resonant excitation of surface slab modes, allowing evanescent wave amplification.

3:06PM D35.00004 Optical Super Lens: from near-field to far field1, XIANG ZHANG, Chancellor’s Professor and Director — Recent theory predicted a new class of meta structures made of engineered sub wavelength entities - meta “atoms” and “molecules” which enable the unprecedented electromagnetic properties that do not exist in the nature. For example, artificial plasma and artificial magnetism, and super lens that focuses far below the diffraction limit. The metamaterials may have profound impact in wide range of applications such as nano-scale imaging, nanolithography, and integrated nano photonics. I’ll discuss a few recent experiments that demonstrated these intriguing phenomena. We showed, for the first time, the high frequency magnetic activity at THz generated by artificially structured “meta molecule resonance”, as well as the artificial plasma. Our experiment also confirmed the key proposition of super lens theory by using surface plasmon. We indeed observed optical superlensing which breaks down so called diffraction limit. I’ll also discuss nano plasmonics for imaging and bio-sensing. The surface plasmon indeed promises an exciting engineering paradigm of “x-ray wavelength at optical frequency.”

1 NSF Nano-scale Science and Engineering Center (NSEC).

3:42PM D35.00005 Surface plasmon polariton bound state and negative index imaging at the dielectric edge, IGOR SMOLYANINOV, BAE Systems, YU-JU HUNG, EHREN HWANG, CHRISTOPHER DAVIS, University of Maryland — Negative refraction of surface plasmon polaritons at the dielectric edge has been studied using near-field and far-field optical microscopy techniques. Edge plasmon polariton state has been observed. Magnified negative index imaging has been demonstrated using a far-field optical microscope. Good agreement between theoretically calculated and experimentally measured images has been demonstrated.
Linear and nonlinear optical devices based on plasmonic negative index metamaterials. 

4:06PM D35.00007 Metaplasmonics and Epsilon-Near-Zero Metamaterials for Optical Nanocircuits, Wave-Bending Tunneling Elements, and Nanoantennas 

4:18PM D35.00008 Quantum Josephson Junction Metamaterials 

4:30PM D35.00009 Experimental realization of a generalized superlens using negative refraction at infrared wavelengths 

4:42PM D35.00010 An Experimental Near-Field Focusing Plate 

4:54PM D35.00011 Radiationless Electromagnetic Interference: Perfect Focusing with Evanescent-Field Plates 

5:06PM D35.00012 Contribution of electric quadrupole resonance in optical metamaterials 

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1Department of Electrical and Computer Engineering, Northeastern University, Boston, Massachusetts 02115, USA
2Supported by AFOSR
3Supported by AFOSR-MURI
4This work is supported by the National Science Foundation.
2:30PM D36.00001 Nanoscale Hydrides in Porous Carbon Scaffolds, JOHN VAJO, HRL Laboratories, Malibu, California, USA — Light element and complex anion hydrides (such as LiH, MgH\(_2\), NaAlH\(_4\), and LiBH\(_4\)) are being studied intensely as reversible hydrogen storage materials for fuel cell powered vehicles because they have high gravimetric and volumetric capacities. However, the rates of dehydrogenation and rehydrogenation of these hydrides are typically much too slow to be compatible with proton exchange membrane fuel cell temperatures. The slow rates originate, at least in part, from the high activation energies for diffusion associated with the ionic and covalent bonds found in these materials. In contrast to metallic systems, ionic and covalent bonds are directional. Thus, the transition states for atomic rearrangement occur in particularly unfavorable bonding configurations. This increases the activation energies for diffusion and results in slow phase transformation and hydrogen sorption kinetics. Overcoming these kinetic limitations has become a critical element in the development of light-metal complex hydrides for practical storage applications. Small quantities of catalytic additives have been shown to greatly improve the rates of hydrogen exchange in MgH\(_2\) and NaAlH\(_4\). Another approach involves formation of nanoscale hydrides by incorporation into nanoporous scaffolds. The small pores of the scaffold limit the sizes of the hydrogenated and dehydrogenated phases and thus the diffusion lengths to nanoscale dimensions. These relatively short diffusion lengths reduce diffusion times and therefore, increase overall rates of hydrogen sorption. The size limitations also result in increased interfacial area between reacting phases, which improves hydrogen capacity retention during cycling. This talk will focus on the preparation, characterization, and hydrogen sorption behavior of LiBH\(_4\), MgH\(_2\), and NaAlH\(_4\) incorporated into nanoporous carbon aerogels.

3:06PM D36.00002 A Study of the Structural and Dynamical Properties of Lithium Borohydride Confined within Nanoporous Framework Structures using Neutron Scattering Investigations, CERIS HAMILTON, MICHAEL R. HARTMAN, University of Michigan, HUI WU, University of Maryland / National Institute of Standards and Technology, TERRENCE J. UDOVIC, National Institute of Standards and Technology, JOHN J. RUSH, University of Maryland / National Institute of Standards and Technology, ADAM F. GROSS, HRL Laboratories LLC. JOHN J. VAJO, HRL Laboratories LLC, THEODORE F. BAUMANN, Lawrence Livermore National Laboratory — Lithium borohydride, LiBH\(_4\), is a complex metal hydride that shows great promise as a hydrogen storage medium with a volumetric hydrogen density of 122 kg H\(_2\)/m\(^3\) and a gravimetric hydrogen density of 18.5 wt. %. We have previously reported on the structural and dynamical properties of neat \(^{7}\)Li\(^{11}\)BH\(_4\) as determined by neutron powder diffraction, neutron vibrational spectroscopy, and quasielastic neutron scattering. Here we report on recent measurements undertaken to investigate the changes in the structural and dynamical properties that are observed when this material is confined within nanoporous structures with pore sizes ranging from 4 nm to 25 nm. These materials exhibit a reduction in the structural transition and melting temperatures, which we associate with a marked decrease in the activation energy for reorientational motions of the [BH\(_4\)]\(^{-}\) tetrahedra.

3:18PM D36.00003 Density Functional Screening of Metal Hydride Reactions\(^1\), KARL JOHNSON, University of Pittsburgh, SUDHAKAR ALAPATI, Carnegie Mellon University, BING DAI, University of Pittsburgh, KI-CHUL KIM, DAVID SHOLL, Georgia Institute of Technology — The on-board storage of hydrogen is one of the most vexing problems associated with the development of viable fuel cell vehicles. Hydrides of period 2 or 3 metals can store hydrogen at high gravimetric and volumetric densities. However, existing hydrides either have unacceptable thermodynamics or kinetics. New materials for hydrogen storage are therefore needed. We demonstrate how first principles density functional theory (DFT) can be used to screen potential candidate materials for hydrogen storage. We have used DFT calculations in conjunction with a free energy analysis to screen over a million reactions involving 212 known compounds. This approach has identified several interesting reaction schemes that have not yet been explored experimentally. We have computed the phonon density of states and used this information to predict the van’t Hoff plots for some of the most promising candidate reactions identified through our modeling. We have also examined the thermodynamics of thin films and nanoparticles for selected metal hydrides by accounting for the surface energies of the films or nanoparticles.

3:30PM D36.00004 Reversible Hydrogen Storage in the Lithium Borohydride – Calcium Hydride Coupled System, FREDERICK PINKERTON, MARTIN MEYER, General Motors Research and Development Center — We report large reversible hydrogen storage in a new coupled system, LiBH\(_4\)/CaH\(_2\), via the reaction 6 LiBH\(_4\) + CaH\(_2\) → 6 LiH + CaB\(_6\) + 10 H\(_2\) having a theoretical hydrogen capacity of 11.7 wt% and an estimated reaction enthalpy of ΔH = 59 kJ/mole H\(_2\). Samples that include 0.25 mole (18.2 wt%) TiCl\(_4\) reproducibly store 9.1 wt% hydrogen, corresponding to 93% of the available hydrogen. H\(_2\) is the only evolved gas detected by mass spectrometry. X-ray diffraction confirms that the sample cycles between LiBH\(_4\) and CaH\(_2\) in the hydrogenated state and LiH and CaB\(_6\) in the dehydrogenated state.

3:42PM D36.00005 Structures and Bonding of Li-B-N-H Quaternary Hydrides, HUI WU, 1. NIST Center for Neutron Research 2. University of Maryland, WEI ZHOU, TERRENCE UDOVIC, JOHN RUSH, TANER YILDIRIM, NIST Center for Neutron Research — Complex metal hydrides are of great interest for hydrogen-storage applications due to their potential high hydrogen capacity. Intense efforts has been made on the Li-B-N-H system, with the discovery of several novel quaternary phases. There have been prior studies investigating the structure of one of these new phases (Li\(_3\)BN\(_3\)H\(_10\)). However, all these studies were undertaken on hydrides without any isotopic enrichment, thus resulted in diffraction data of limited quality and yielded structures with questionable bond lengths and unit cell structures determined anion groups. So far, no studies have been reported on the isotopically labeled samples, which are necessary to determine correct structures for these hydrides. We report for the first time the crystal structures of Li\(_2\)BN\(_2\)H\(_4\) and Li\(_4\)BN\(_3\)H\(_4\) derived from high-resolution neutron diffraction data on samples labeled with \(^{1}\)Li, \(^{11}\)B, and D. Our refined structures clarify the prevailing structural discrepancies. We also report corresponding neutron vibrational spectra combined with first-principles calculations to gain more insight between structure and bonding. The configurations of both BH\(_3\) and NH\(_3\) anions and the structural variations upon compositional changes will be discussed. Our study provides implications to the mechanisms of hydrogen absorption/desorption in these complex hydrides.

3:54PM D36.00006 Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures\(^1\), DONALD SIEGEL, Ford Motor Company, C. WOLVERTON, Northwestern University, V. OZOLINS, University of California at Los Angeles — We propose a set of thermodynamic guidelines aimed at facilitating more robust screening of hydrogen storage reactions. The utility of the guidelines is illustrated by reasessing the validity of reactions recently proposed in the literature and through vetting a list of more than 20 candidate reactions based on destabilized LiBH\(_4\) and Ca(BH\(_4\))\(_2\) borohydrides. Our analysis reveals several reactions having both favorable thermodynamics and relatively high hydrogen densities (ranging from 5–9 wt % H\(_2\) and 85–100 g H\(_2\)/l), and demonstrates that chemical intuition alone is not sufficient to identify valid reaction pathways.

\(^1\)DOE Metal Hydride Center of Excellence

\(^{2}\)Does Metal Hydride Center of Excellence
Crystallography of the Perovskite-type Hydride NaMgH₃. TERRENCE UDOVIC, HUI WU, WEI ZHOU, JOHN RUSH, TANER YILDIRIM, NIST Center for Neutron Research, Gaithersburg, MD 20899 — The crystal structure, lattice dynamics, and local metal-H binding configuration of the perovskite hydride NaMgH₃ were investigated using combined neutron powder diffraction, neutron vibrational spectroscopy, and DFT calculations. NaMgH₃ crystallizes in the orthorhombic GdFeO₃-type perovskite structure (Pnma) with α-β-α octahedral tilting in the temperature range of 4-370 K. In contrast with previous structure studies, the refined Mg-H lengths and H-Mg-H angles indicate that the MgH₂ octahedra maintain a near ideal configuration, which is corroborated by both valence methods and our DFT calculations, and is consistent with perovskite oxides with similar tilt factor values. The temperature dependences of the lattice distortion, octahedral tilting angle, and atomic displacement of H are consistent with the recently observed high H mobility at elevated temperatures. The stability and dynamics of NaMgH₃ are discussed and rationalized in terms of lattice distortion, cation octahedra tilting, and local bonding configurations in the observed perovskite structure. Further experiments reveal that its perovskite crystal structure can be used to improve the slow hydrogenation kinetics of some strongly bound light-metal-hydrate systems such as MgH₂ and to design new alloy hydrides with desirable hydrogen-storage properties.

Bonding changes in compressed NaBH₄ probed by inelastic X-ray scattering1. ANDREW CORNELIUS, RAVHI KUMAR, MALCOLM NICOL. University of Nevada, Las Vegas, MICHAEL HU. HPCAT and Carnegie Institution of Washington, PAUL CHOW. Argonne National Laboratory — Hydrogen storage for commercial applications is an ongoing challenge in materials science research in recent years. Complex borohydrides are technologically promising materials due to their light weight and high gravimetric and volumetric hydrogen density. So far knowledge of the structural and bonding changes in these systems is elusive due to low z elements and lack of in-situ experimental probes. Here we present the first experimental results of boron K-edge inelastic X-ray scattering performed on NaBH₄ revealing the nature of bonding changes during compression up to 12 GPa. NaBH₄ undergoes structural phase transition from cubic (Fm-3m) to tetragonal (P421/c) above 6 GPa and to orthorhombic (Pnma) above 8.3 GPa. The high pressure tetragonal and orthorhombic phases show weakening of B-H bonding during phase transition. Further, NaBH₄ may be considered as a representative example for isostructural systems since a similar structural sequence is also observed in KBH₄ on compression. The experimental details and the inelastic x-ray scattering results will be presented.

On the Formation of LaFe₃H₈. JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Formation of a LaFe₃H₈ hydride is explored by means of density functional theory. Enthalpies of formation ∆H with respect to the elemental metals and H₂ are calculated for various hydrogen configurations in four prototype crystal structures. We find ∆H < 0 in many cases, suggesting the existence of LaFe₃H₈, as does Miedema's semi-empirical model. ∆H is a minimum for the LaFe₃H₈ stoichiometry with hydrogen occupying the 4e, 8g, and 16m sites in the orthorhombic Cmcm structure. Phonon dispersion relations and elastic constants computed for that structure exhibit no anomalies, demonstrating vibrational stability. Similar results for LaFe₅ indicate that compound may form under pressure.

Magnetooptic Ellipsometry: Determination of free charge carrier properties in semiconductor device structures1. MATHIAS SCHUBERT, TINO HOFMANN. Dept. of Electrical Engineering and Nebraska, University of Nebraska-Lincoln — The standard tool for the electrical characterization of free charge properties in semiconductor layer structures is the electrical Hall effect. However, besides the requirement for electrical contacts, the application of this technique to investigate complex heterostructures is very difficult and reliable deconvolution of the individual layer contributions to the measured Hall-Voltage virtually impossible. In our contribution we show that magnetooptic ellipsometry at long wavelengths when applied to conducting or semiconducting multilayer structures can yield equivalent and even much increased information. Our technique allows the independent measurement of free charge carrier density, type, mobility, and effective mass including anisotropy without any electrical contact in buried structures, and which may have been inaccessible to any true electrical evaluation thus far. We present results for multilayer AlGaP and GaInP samples with different doping concentrations. Furthermore, multilayer LED device structures were investigated and we demonstrate that magnetooptic ellipsometry allows deconvolution of the individual free charge carrier contributions of the p- and n-type regions of the device structure. We predict a realm of applications for magnetooptic ellipsometry in future materials research and engineering.

Cyclotron mass of two-dimensional holes in (100) oriented GaAs/AlGaAs heterostructures. T.M. LU, Z.F. LI, D.C. TSUI, Princeton University, M.J. MANFRA, L.N. PFEIFFER, K.W. WEST. Bell Laboratories — We have measured the microwave cyclotron resonance of low-density two-dimensional hole gases in (100) oriented heterostructures, including single interface heterostructures (SiHs) and 20nm-wide quantum wells(QWs). It was found that in the case of the SiHs, the cyclotron mass is relatively insensitive to the hole density, ranging from 0.25 x 10¹⁰/cm² to 1.31 x 10¹⁰/cm², and has a value of approximately 0.5mₑ. On the other hand, for holes in the QWs, the cyclotron mass decreases from 0.48mₑ at density $p = 6.9 	imes 10^{10}$/cm³ to 0.29mₑ at $p = 0.8 	imes 10^{10}$/cm³. In this talk, the absorption spectra will be shown, and a qualitative explanation will be presented.

High-Gap Semiconductors and Their Absorption Mechanisms at Millimeter and Submillimeter Wavelengths. J.M. DUTTA, C.R. JONES, North Carolina Central University, V. PARSHIN, Applied Physics Institute, RAS, B. GARIN, V. POLYAKOV, A. RUKOVISHNIKOV, Institute of Radio Engineering & Electronics, RAS — Experimental data has been applied to extend the available theoretical models to elucidate the predominant mechanisms of absorption for mm and sub-mm electromagnetic waves in high-gap semiconductors, especially CVD diamond and SiC, which are among the most promising low-loss materials commercially available. Dielectric properties of CVD diamonds, as measured by several laboratories, over a wide range of temperature and frequency will be discussed. The experimental data gathered, both from dielectric and electrical measurements, has been applied to extend available theoretical models for CVD diamonds. Similar studies are undertaken on SiC to determine the primary loss mechanisms for SiC in the mm wavelength range. Preliminary experimental results will be presented.

Propagation of light in birefringent tilings. ANGELO MASCARENHAS, BRIAN FLUEGEL, LEKHNATH BHUSAL, National Renewable Energy Laboratory — Two-dimensional tilings of an optically birefringent material are proposed as an orientational superlattice for light. The light modes that result from loss-free refraction are analyzed. It is shown that the behavior for light propagation in such lattices leads to totally bound as well as propagating states. The behavior of light propagation in several such tilings is compared.
Properties of Bulk GaN Crystals grown from the Solution, MADHU MURTHY, George Mason University, Fairfax, VA. JAIME A. FREITAS JR., MICHAEL A. MASTRO, RACHEL M. FRAZIER, Naval Research Laboratory, Washington DC.

3:18PM D37.00005 — WE investigated the structural and optical properties of bulk GaN single crystal grown from solution at temperatures < 900°C and a pressure of ~ 0.3 MPa. The X-ray diffraction peaks measured on both Ga- and N-face of the epitaxial film are 34.561 and 34.612 arcsec, respectively, which are two orders of magnitude lower than the substrate. The photoluminescence measurements performed on both faces of the sample, showed a dominant intense emission near 3.47 eV, which is assigned to recombination process involving shallow impurities and excitons. The two additional bands observed at 3.25 eV and 2.25 eV are assigned to donor-acceptor recombination process and the yellow band, respectively. The relative intensities of these bands intensities suggest a reduction of the concentration of defects incorporated in the epitaxial film, as compared with the substrate. These variations are consistent with different incorporation rate of point defects at different crystal surface polarity.

1 This work was partially supported by the Office of Naval Research. M. Murthy is supported by NSF Award # ECS-0330226.

3:30PM D37.00006 — D.Y. SONG, A. CHANDOLU, L. TIAN, N. STOJANOVIC, S.A. NIKISHIN, M. HOLTZ, Texas Tech University — Selective area growth (SAG) is useful for overcoming mismatch between non-native substrates and epitaxial materials. SAG of GaN is carried out using metalorganic chemical deposition with silicon dioxide as the mask material with openings ranging from 500 nm to several microns. This talk addresses optical properties of completed GaN pyramidal islands grown using SAG. SEM-based cathodoluminescence (CL) is used to investigate the bandgap emission. The optical properties at different positions on the pyramids are related to overgrowth conditions which determine the luminescence properties. The apex region is almost fully relaxed, while the pyramid base exhibits a red-shifted CL spectrum. This shift is attributed to stress and impurity incorporation in the overgrown sidewall region. The red shift observed in CL spectra on the pyramid sidewall region gradually increases from apex to base, varying by ~ 40 meV, when they exceed the size of the opening in the silicon dioxide mask. However, the pyramid has almost uniform luminescence properties when overgrowth does not occur. The CL line width is narrowest at the pyramid apex, suggesting a decrease in the disorder density. The authors acknowledge support from the National Science Foundation (ECS-0609416 and ECS-0304224) and the J. F Maddox Foundation.

3:42PM D37.00007 — JOSEPH BRADLEY, GERALD SEIDLER, University of Washington, RAFAEL DALMAU, North Carolina State University, KENNETH NAGLE, University of Washington, ZLATKO STAR, North Carolina State University — A fundamental description of the mechanisms underlying the diverse applications of w-AlN requires a complete understanding of its short-range and long-range electronic structure. Here, we report momentum-transfer (q) dependent nonresonant inelastic x-ray scattering (NRIXS) measurements of single crystal w-AlN, surveying the low-energy plasmon regime, as well as the complex behavior at the Al K and L edges. This complete determination of the dynamic structure factor S(q,w) over a wide range of q and w both within and perpendicular to the basal plane allows for a uniquely detailed perspective on chemical bonding and low-energy electronic response in w-AlN. Our results are compared and contrasted with two independent ab initio theoretical treatments.

3:54PM D37.00008 — A. SEDHAIN, N. NEPAL, M.L. NAKIRMI, J.Y. LIN, H.X. JIANG, Department of Physics, Kansas State University, J.H. EDGAR, Department of Chemical Engineering, Kansas State University — Polar and non-polar AlN homo- and hetero-epitaxial layers were grown on sapphire and AlN substrate materials by metal organic chemical vapor deposition. Polarization resolved deep ultraviolet photoluminescence (PL) spectroscopy was employed to investigate the optical properties of these samples. For the first time, B and C valence band related free exciton (FX) transitions without a dominant S(0) polarization were directly observed from PL. The emission energy peaks of B and C excitons were found to locate at 199 and 212 meV higher than that of the A-exciton transition position possessing the Ec polarization. A more comprehensive picture of the valence band structure of AlN is thus directly observed from PL measurements. AlN homo-epilayers in all orientations (a-, c-, and m-plane) were found to be strain free and have a nearly identical band gap of 6.099 eV at 10 K. The band edge peak intensity ratios of a-, c-, and m-plane homo-epilayers were roughly 32.5:1 and line width was found to be the smallest in a-plane homo-epilayer. Our results also indicated that built-in electric fields are almost absent in all AlN homo-epilayers.

4:06PM D37.00009 — NIELS E. CHRISTENSEN, Dept. of Physics and Astronomy, University of Aarhus, DK-3000 Aarhus, Denmark, ROBERT LASKOWSKI, Inst. of Materials Chemistry, Techn. University of Vienna, A-1060 Vienna, Austria — First-principles calculations based on solution of the Bethe-Salpeter equation of excitons in the high-pressure AlN phase show that a delocalization-localization transition occurs as applied pressure. The transition, which is associated with a sudden increase in exciton binding energy, is related to a pressure-induced rearrangement of the energy bands.

4:18PM D37.00010 — WAN-TSANG WANG, Department of Physics, Center of Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan — The wurtzite bulk inversion asymmetry (WBIA) terms in the k·p Hamiltonian have been derived from the linear combination of atomic orbital method, and the analytic form of Dresselhaus effect is obtained via an eight-band k·p Hamiltonian. It is found that WBIA terms lead to not only a spin-degenerate line (along the kz axis) but also a minimum-spin-splitting surface. Furthermore, they can induce large spin splitting energies in wide-gap wurtzite materials such as GaN. Consequently, the D’yakonov-Perel’ (DP) spin-relaxation mechanism can be effectively suppressed for all spin components in the [001] wurtzite quantum wells (QWs) at a resonance condition through appropriate sample design or the application of a suitable gate bias. Therefore, wurtzite QWs (e.g., InN/GaN or AlN) are potential candidates for spintronic devices such as the resonance spin lifetime transistor.

4:30PM D37.00011 — D. Y. SONG, P. PANDIT, A. CHANDOLU, M. BASAVARAJ, S.A. NIKISHIN, M. HOLTZ, Texas Tech University — The intrinsic phonon decay properties of high-quality crystalline III-nitrides are found to be critical to device self-heating. As well as for understanding the properties of phonons, micro-Raman scattering and piezoelectric studies of the Al(1)(TO), E(2)(TO), E(2)(LO), and A(1)(LO) symmetry phonons of GaN and the A(1)(TO), E(2)(TO), E(2) and A(1)(LO) symmetry phonons of AlN from 13 to 375 K. By applying anharmonic decay theory to the observed temperature dependences of the phonon energies, the phonon decay mechanisms of these center-energy vibrations have been determined. Thermal expansion is taken into account in using published temperature-dependent coefficients. Both GaN and AlN A(1)(TO) and E(2)(TO) vibrations are described by symmetric two-phonon decay. The GaN E(2) decays via creation of three phonons, however, the AlN E(2) decays symmetrically into two phonons. The GaN and AlN LO bands are interpreted by an asymmetric two-phonon decay. Phonon lifetimes are obtained based on the observed linewidths, and the dependence allows us to estimate the intrinsic phonon lifetime for each vibration. The authors acknowledge support for this work by the National Science Foundation (ECS-0609416 and ECS-0304224) and the J. F Maddox Foundation.

4:42PM D37.00012 — ABSTRACT WITHDRAWN —
The use of classical interatomic potentials. An embedded atom method (EAM) potential for titanium-vanadium is presented, and thermodynamic and mechanical properties of this alloy are calculated using the potential. The results are compared to density functional theory results and experimental results when available.

Vanadium is an important alloying element for titanium since its addition stabilizes the high temperature bcc phase of titanium at lower temperatures, and bcc-stabilized titanium alloys generally showed improved hardness and applications due to their large strength-to-weight ratio and their ability to resist corrosion. Vanadium is an important alloying element for titanium since it stabilizes the high temperature bcc phase of titanium at lower temperatures, and bcc-stabilized titanium alloys generally showed improved hardness and formability [1].

Titanium-vanadium is also a reasonable starting point in the study of more complex titanium alloys of commercial importance. The calculation of many alloy properties requires the use of large numbers of atoms simulated over long periods of time. These calculations are currently only feasible through the use of classical interatomic potentials. An embedded atom method (EAM) potential for titanium-vanadium is presented, and thermodynamic and mechanical properties of this alloy are calculated using the potential. The results are compared to density functional theory results and experimental results when available.

The effect could play a role in the observed efficiency droop of LEDs and play a major role in the limitations of GaInN/GaN laser diodes. This work was supported by DOE/NETL.

Monday, March 10, 2008 2:30PM - 5:30PM — Session D38 DCMP: Metals: Defects and Elastic Properties Morial Convention Center 230

2:30PM D38.00001 Atomic short-range order effects on magnetostriction in Fe-rich Fe-Ga . YEVGENIY PUZYREV, G. E. ICE, G. M. STOCKS, Oak Ridge National Laboratory, R. MCQUEENEY, Ames National Laboratory, YINGZHOU DU, Iowa State University — We have measured diffuse x-ray scattering from an Fe-rich Fe-Ga BCC single crystal. Measurements were made on beamline 33-ID at the Advanced Photon Source using a wavelength dispersive spectrometer to suppress Compton, Fluorescence and Resonant Raman backgrounds. Data was collected over a large volume in reciprocal space and measurements were made at two energies to maximize and minimize the x-ray scattering contrast between Fe and Ga. We recovered short-range order (SRO) parameters for the crystal. Using these SRO parameters we use KKR-CPA and locally self-consistent multiple scattering (LSMS) calculations to study the effects of local atomic environment on electronic and magnetic structure of the alloy. Research sponsored by the Division of Materials Sciences and Engineering.

2:42PM D38.00002 First-principles study of helium bubble formation at a palladium lattice vacancy . PEI LIN, YAN WANG, MEI-YIN CHOU, Georgia Institute of Technology — Helium (4He) generated from the tritium decay is one of the main reasons for macroscopic radiation damage in the structural components of nuclear devices such as fission reactors and tritium storage media. In contrast to the hydrogen isotopes, helium with its closed electron shell is inert inside metals and tends to aggregate into bubbles which can cause deterioration of materials and influence the lifetime of reactor components. To examine this behavior, we have performed ab initio calculations of helium atoms inside palladium (Pd) using density functional theory (DFT) and the projector augmented wave (PAW) method within the generalized gradient approximation (GGA). We find that He diffuses easily in a defect-free Pd lattice. However, it is energetically favorable for multiple He atoms to be trapped at an isolated Pd vacancy site, forming a cluster of up to 8 atoms. The atomicistic mechanisms of He-vacancy interaction in Pd are investigated by studying the corresponding electronic structural properties.

2:54PM D38.00003 Embedded Atom Method Potential for Titanium-Vanadium Alloys1 . MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University, Department of Physics — Titanium alloys are important materials for aerospace applications due to their high strength-to-weight ratio and their ability to resist corrosion. Vanadium is an important alloying element for titanium since it stabilizes the high temperature bcc phase of titanium at lower temperatures, and bcc-stabilized titanium alloys generally showed improved hardness and forgeability [1]. Titanium-vanadium is also a reasonable starting point in the study of more complex titanium alloys of commercial importance. The calculation of many alloy properties requires the use of large numbers of atoms simulated over long periods of time. These calculations are currently only feasible through the use of classical interatomic potentials. An embedded atom method (EAM) potential for titanium-vanadium is presented, and thermodynamic and mechanical properties of this alloy are calculated using the potential. The results are compared to density functional theory results and experimental results when available.

1Supported in part by the DOE. Computing resources provided by OSC and NERSC.
3:06PM D38.00004 Atomistic dislocation simulation of aluminum using a tight-binding method, CHEE GAN, Institute of High Performance Computing, Singapore, SIU-SIN QUEK, Institute of High Performance Computing — Atomistic simulation of dislocation in aluminum has been performed using a tight-binding method where the parameters are based on the works of Mehl and Papaconstantopoulos at the Naval Research Laboratory. We study the dissociation of a perfect edge dislocation (the dislocation line is along the [112] direction) of Burgers vector of $\frac{a}{2}[10\bar{1}]$ into two partials of $\frac{a}{2}[\bar{2}1\bar{1}]$ and $\frac{a}{2}[\bar{1}2\bar{1}]$ on the (111) slip plane. By performing a large scale atomistic relaxation, we observe a separation of partials of about 14 Å and a stacking fault region. We will comment on the estimate of partials separation predicted by the elasticity theory, which relates to certain quantities such as the stacking fault energy.

3:18PM D38.00005 First-principles calculation of dislocation properties of ductile rare-earth intermetallic compounds, MIN JI, CAI-ZHUANG WANG, Ames Laboratory, US DOE, Ames, IA 50011, USA, KAI-MING HO, Ames Laboratory, US DOE, Ames, IA 50011, USA and Department of Physics, Iowa State University, Ames, IA 50011, QIAN CHEN, XIANG-YANG LIU, BULENT BINER, Ames Laboratory, US DOE, Ames, IA 50011, USA — We have used first-principles calculations to study the mechanical properties of rare-earth intermetallic B2 compounds which exhibit significant ductility. According to Peierls-Nabarro model and slip plane observed in tensile experiments, we have calculated and compared the 110 gamma surface energy for both brittle NiAl and ductile YCu. We also compared unstable stacking fault and twinning energy for a series of B2 compounds with different ductility. Correlation between these energetics and the ductility are discussed.

3:30PM D38.00006 Effect of Chemistry on Dislocation Core Properties in α-Fe: AB INITIO-BASED APPROACH, ZHENZHENG CHEN, NICHOLAS KIOUSSIS, Dept. of Physics, California State Univ., Northridge, NASR GHONIEM, Dept. Mechanical and Aerospace Engr., UCLA, TADASHI HASEBE, Dept. of Mechanical Engr., Kobe Univ., Japan — Screw dislocations in α-Fe and its alloys play an important role on the low-temperature mechanical property. The solute atom can cause a significant local reconstruction of the dislocation core and therefore affect the mobility. Since direct investigations of the solute-dislocation interaction by first principles calculation remains a difficult problem, we employ a hybrid coupling approach that includes atomistic dislocation modeling with ab initio parameterization of the inter-row interactions, proposed by Suzuki. Using this approach, we have investigated the change of core structure and the $a/2[11\bar{1}]$ screw dislocation mobility induced by impurities of Cu and Cr. We find that Cu induces a change from a non-degenerate (P=0, where P is the core polarization) core structure in α-Fe to a degenerate (P=1) one, while Cr impurity does not change the P at any concentration. We have also studied the behavior of these systems under stress, and found that Cr impurities lower the mobility of the screw dislocation, while Cu induces that the dislocation of Fe-Cu system under stress exhibits a peculiar stable $\rightarrow$ metastable $\rightarrow$ stable transition, and strengthens α-Fe. The above conclusions are supported by molecular dynamics calculation, which also show that Cu impurities, in addition to changing the core polarization, dramatically increase the edge components of screw dislocation in Fe.

3:42PM D38.00007 Dependence of the Strain Rate Sensitivity of Crystalline Materials on the Distribution of Obstacles to Dislocation Motion, RENGE LI, ZHIJIE XU, CATALIN PICU, Rensselaer Polytechnic Institute — The strength and strain rate sensitivity of metals is usually described in terms of the concentration of obstacles to dislocation motion, i.e. the mean of the obstacle spatial distribution function. In this study we investigate the role of higher moments of this distribution function on these parameters. It is shown that large local fluctuations of obstacle density influence to a large extent the strain rate sensitivity of the material, while the effect on the strength (critical resolved shear stress) is smaller. It is shown that a large reduction of the strain rate sensitivity is associated with a change in the dislocation motion mode from smooth to jerky. Populations composed from obstacles of same strength but different activation energy, as well as obstacles of same activation energy and different strength are also studied.

3:54PM D38.00008 Elastic properties of γ-Pu by Resonant Ultrasound Spectroscopy, IZABELA STROE, Los Alamos National Laboratory, A. TRUGMAN, J. BETTS, A. MIGLIORI, C. H. MILEKE — Despite of intense experimental and theoretical work on Pu, there is still little understanding of the strange properties of this metal. We used resonant ultrasound spectroscopy method to investigate the elastic properties of pure polycrystalline Pu at high temperatures. Shear and longitudinal elastic moduli of the γ-phase of Pu were determined simultaneously and the bulk modulus was computed from them. A smooth linear and large decrease of all elastic moduli with increasing temperature was observed. We calculated the Poisson ratio and found that it increases from 0.242 at 519K to 0.252 at 571K.

4:06PM D38.00009 The 50 K anomaly in the shear modulus of β-PdH$_{0.71}$, DOUGLAS SAFARIK, RICARDO SCHWARZ, Los Alamos National Laboratory — When palladium hydride, PdH$_x$, is rapidly cooled to liquid helium temperature and then slowly reheated, both the heat capacity and electrical resistivity show a peak in the range 50 < T < 80 K, depending on the composition x. This “50 K anomaly” has been previously explained in terms of formation of long-range ordered hydrogen superlattice structures. However, several aspects of the 50 K anomaly are inconsistent with an ordering phase transition, namely, the temperature of the anomaly depends on the rate of cooling, and the magnitude of the anomaly is larger for a fast cooling rate than for a slow cooling rate. We have studied the 50 K anomaly by measuring the elastic constants of single-crystal PdH$_{0.71}$ in the temperature range 1.4 < T < 300 K during both fast cooling and slow warming. During warming, we observed a peak in the shear modulus $C'' = (C_{11} - C_{12}/2)$ at 55 K, which we attribute to the 50 K anomaly. In contrast, we observed no peak in the temperature dependence of the shear modulus $C_{14}$ or of the bulk modulus $B$. We propose that the 50 K anomaly arises not from the formation of long-range ordered hydrogen superlattice structures, but from freezing of the hydrogen short-range order as the hydride is cooled.

4:18PM D38.00010 Field theoretical approach to deformation dynamics, SANICHIRO YOSHIDA, Southeastern Louisiana University — Based on a recent gauge theory called physical mesomechanics, an attempt is made to formulate the deformation dynamics of solid-state materials comprehensively. In this formalism, deformation is described as a linear transformation of the position vector connecting two nearby points of the material; the transformation is global in the elastic regime and local in the plastic regime. The demand of local invariance leads to a Maxwell-type field equation, in which a symmetry charge analogous to the electric charge is defined. Dynamics in the plastic regime is characterized by transverse force proportional to rotational displacement, as opposed to translational displacement in the elastic regime, and longitudinal force proportional to velocity. The transverse force is a restoring force, which can be interpreted as the recoverability mechanism that the material regains in the plastic regime. The longitudinal force can be interpreted as a field force acting on the above-mentioned charge, which is basically an energy-dissipating force causing the irreversibility of plastic deformation. Fracture is considered to be the situation where the material completely loses recoverability. Supporting experimental data will be presented.
4:30PM D38.00011 Where is the Simple Hexagonal Structure in Tin?1, MICHAEL MEHL, DANIEL FINKENSTADT2. Naval Research Laboratory — The heavier elements of periodic table column IV exhibit number of structural phase transitions under pressure. Si and Ge transform from the ground-state diamond structure to, successively, the β-Sn structure, a body-centered orthorhombic structure, the simple hexagonal structure, etc., ending at a close-packed phase (fcc or hcp) near 200 GPa. Tin also transforms from diamond to β-Sn, but then to a body-centered tetragonal phase, ending with the body-centered cubic phase. The simple hexagonal phase is not seen, despite the fact that numerous tin-rich alloys exhibit a simple hexagonal structure. To understand this we performed DFT calculations on tin in various crystal structures, using both full-potential LAPW and VASP with a PAW potential. Surprisingly, we find that the simple hexagonal phase is degenerate with a simple hexagonal structure. To understand this we performed DFT calculations on tin in various crystal structures, using both full-potential LAPW and tetragonal phase, ending with the body-centered cubic phase. The simple hexagonal phase is not seen, despite the fact that numerous tin-rich alloys exhibit a simple hexagonal structure, etc., ending at a close-packed phase (fcc or hcp) near 200 GPa. Tin also transforms from diamond to β-Sn over pressures at which the β-Sn phase is seen experimentally. This holds both for LAPW and VASP calculations, in both the LDA and the GGA. We explore reasons for the lack of a tin simple hexagonal phase, including zero point and spin-orbit effects.

1Supported by the Office of Naval Research. Computational support from the DoD HPCMO.
2NRC Postdoctoral Fellow

4:42PM D38.00012 Ab initio study of Fe-rich Fe-Cu alloys1, DAVID REITH, RAIMUND PODLOUCKY, Department of Physical Chemistry, University of Vienna — Cu precipitates are important for strengthening steel. Our ab initio study aims to model the thermodynamical stability of Cu precipitations in α-Fe. As a first step, a density functional theory (DFT) supercell approach is applied to study Fe_{1-x}Cu_x alloys at small concentrations x. From the DFT total energies a strongly nonbonding substitutional energy E_{sub} ≈ 0.7 eV is derived, which is significantly larger than results of a previous DFT study [1]. Based on force constants derived by the same DFT approach the temperature dependent vibrational free energy is determined [2]. In particular at higher temperatures the vibrational entropy significantly reduces the formation energy. Finally, by using the entropy of mixing the dilute Fe-Cu alloy becomes stabilized. The derived phase diagram is in good agreement with experimental data [3]. According to our analysis, the vibrational free energy is very important for a correct modelling of the phase stability of Fe-rich Fe-Cu alloys. [1] C. Domain et al., PRB, 65, 024103 (2001) [2] D. Alfe et al, PRB, 65, 045123 (2001) [3] B. Predel, Landolt-Börnstein - IV, Springer, Volume 5d (1994)

3Work supported by FWF project nr. P18480

4:54PM D38.00013 Strain-induced interactions in size-mismatched alloys: A Kanzaki force approach1, ALEJANDRO DIAZ-ORTIZ, OLEG SCHIGYLO, VLADIMIR BUGAEV, HELMUT DOSCH, ALEXANDER UDYANSKY, HARALD REICHERT, Max Planck Institute for Metals Research, RALF DRAUTZ, Department of Materials, University of Oxford — A perturbative approach to determining the strain-induced effective interactions in binary alloys with large atomic-size mismatch is presented. Using the chemical energy as the reference state, the strain-induced energy of the alloy is cast into a many-body (Kanzaki) force expansion that depends on both the configurational and displacive degrees of freedom. It is shown that the k-space energy expansion is valid for all wave-lengths. The theory is then applied to the Cu_{13}Au alloy where, due to the large difference among atomic sizes, considerable relaxations are observed from first-principles calculations. We found that the inhomogeneous contribution (k≠0) dominates the strain energy in Cu_{13}Au, whereas the homogenous part (k=0), notwithstanding its configurational dependence, contributes only a few percent.

1Work supported by the Alexander von Humboldt Foundation.

5:06PM D38.00014 New candidates for the Pt_{33}Ti structures in intermetallics, ERIN GILMARTIN, JACQUELINE CORBITT, GUS HART, Brigham Young University — The only known intermetallic structure with an 8:1 stoichiometry is that of Pt_{33}Ti. Because of its uniqueness, this structure has been studied in Pt, Pd, and Ni rich systems. However, these metals have only been paired with a handful of other elements. Are there more elements that when alloyed with Pt, Pd, or Ni order with the Pt_{33}Ti structure? We explored 40 different Pd- and Pt-based binary systems. We calculated their formation enthalpies for the Pt_{33}Ti structure. Compared to the value in the tie line between pure Pd/ Pt and experimentally-observed ground states. We find that there are other (beyond those experimentally observed) possible alloys with this structure. These new Pt/Pd-rich alloys could fin application in the jewelry and catalysis industries.

5:18PM D38.00015 Properties of the type I Ge-based clathrates Ba_{x}Al_{13}Ge_{33} and Ba_{x}Al_{16}Ge_{30}, EMMANUEL NENGHABI, Texas Tech University, CHARLES MYLES, Texas Tech University — The type I clathrate lattice is simple cubic with 46 atoms per unit cell. The cages in this lattice can host “guests” and the framework can have substituted atoms. Here, we focus on the “alloy” system Ba_{x}Al_{13}Ge_{33-x} (x is an integer; 0<x<15). The Ba are guests and Al substitutes for some Ge framework atoms. Using the local density approximation (LDA), we have calculated some properties of the type I clathrates Ba_{2}Al_{13}Ge_{31} and Ba_{2}Al_{16}Ge_{30}. Our calculations of the equilibrium structures predict that Ba_{2}Al_{13}Ge_{31} and Ba_{2}Al_{16}Ge_{30} have approximately the same lattice constant and that Ba_{2}Al_{13}Ge_{31} is expected to be slightly more stable than Ba_{2}Al_{16}Ge_{30}. Our band structures and electronic density of states results predict that Ba_{2}Al_{13}Ge_{31} is metallic and that Ba_{2}Al_{16}Ge_{30} is a semiconductor with an indirect fundamental band gap of 0.3 eV. The vibrational spectrum predicts low frequency rattling modes caused by the Ba guests that are loosely bound in the Al-Ge framework cages. Such modes may scatter the heat-carrying acoustic vibrational framework modes, potentially reducing the thermal conductivity.

Monday, March 10, 2008 2:30PM - 5:30PM - Session D39 GSNP: Focus Session: Econophysics and Applications Outside of Physics - Morial Convention Center 231

2:30PM D38.00001 Image Segmentation in Linear Time using the Potts Model. FRANK W. BENTREM, Marine Geosciences Division, Naval Research Laboratory, Stennis Space Center, Mississippi 34552 — A computational method is described which efficiently segments digital grayscale images using the Q-state Ising (or Potts) model. Since the Ising model was first proposed in 1925, physicists have studied lattice models to gain deep insights into ordered/disordered systems. Some researchers have realized that digital images may be modeled in much the same way as these physical systems (i.e., as a square lattice of numerical values). A major drawback in using this technique for image segmentation is that it processes in exponential time. Advances have been made via certain approximations to reduce the segmentation process to power-law time. However, real-time processing (such as for sonar imagery) requires much greater efficiency. We describe an energy minimization technique using four Potts (Q-Ising) models which processes in linear time. The technique is demonstrated on acoustic seafloor images as well as medical images.
2:42PM D39.00002 Battles between an insurgent army and an advanced army - focus on strategy. SURAJIT SEN, LINDA SHANAHAN, Physics Dept, SUNY-Buffalo — Detailed and aggregate analyses of the outcome of past battles focusing on rates of troop losses or on the ratios of forces on each side is at the heart of present knowledge about battles. Here we present non-equilibrium statistical mechanics based studies of possible outcomes of well matched strategic battles by a “blue” army against insurgency based attacks by well matched opponents in a “red” army in red territory. We assume that the red army attacks with randomly varying force levels to potentially confuse and drive the blue’s strategies. The temporal evolution of the model battles incorporate randomness in the deployment of the reds and hence possess attendant history dependence. Our results reveal that while unpredictable events play a major role in battles, a balance between risk of exposure in a battlefield and the use of short range intelligence is needed in determining whether one side can decimate the other, and hence force a battle to end.

1Research supported by Army Research Office.

2:54PM D39.00003 Understanding individual human mobility patterns, MARTA C. GONZÁLEZ, Northeastern University, CESAR A. HIDALGO, Notre Dame University, ALBERT-LÁSZLO BARABÁSI, Northeastern University and Notre Dame University — Understanding human mobility patterns is of major importance for a number of areas, ranging from urban planning to traffic forecasting, transportation geography, and preventing the spread of biological and mobile viruses. Yet, in the absence of tools to monitor the time resolved location of a large number of individuals, our understanding of the basic laws governing human trajectories remains limited. Here we study the individual mobility pattern of mobile phone users whose position is tracked in a time resolved manner. We find that the displacement distribution of the whole population can be approximated with a truncated Lévy statistics, in agreement with earlier measurements. We show, however, that the main contribution to the observed distribution comes from the differences in the travel pattern of individuals. Furthermore, we find that the individual trajectories are bounded in space and are highly anisotropic, an effect that increases with the trajectory’s radius of gyration. After we correct for differences in the radius of gyration and anisotropy all individuals are described by the same universal mobility pattern. These results open new avenues for modeling human motion, with important impact on agent based modeling, epidemic prevention, emergency response and urban planning.

3:06PM D39.00004 Epidemics with Multistrain Interactions: Cross Immunity and Antibody-Dependent Enhancement. SIMONE BIANCO, LEAH SHAW, College of William and Mary — Dynamics of epidemic spread is a problem of global interest. In this work we investigate the dynamical properties of a multistrain disease in a population where the strains interact via antibody-dependent enhancement (ADE) and cross immunity. ADE is a property of some multistrain diseases, such as dengue fever and Ebola, in which the antibodies generated by a primary infection with a strain tend to increase the infectiousness of a secondary infection with a different strain. After a primary infection, cross immunity provides temporary reduced susceptibility to the other strains. The presence of chaotic outbreaks and desynchronization between strains has already been observed in a model with no cross immunity if the ADE is sufficiently strong. The addition of weak cross immunity provides a stabilizing effect, while strong cross immunity leads to large amplitude chaotic outbreaks. A stochastic version of the model is also considered.

3:18PM D39.00005 Panic reactions and global disease dynamics. RAFAEL BRUNE, CHRISTIAN THIEMANN, Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany, BERND BLASIUS, ICBM Oldenburg, Germany, THEO GEISEL 1, DIRK BROCKMANN, Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany — We analyze spatially extended disease dynamics in a system in which individuals change their dispersal characteristics in response to the local infection level. The key question is to what extent infectious wave front dynamics and the time course of the global infection change in response to host awareness and individuals trying to avoid infection by increased dispersal. We investigate two qualitatively different responses to the local degree of infection. In one system (panic reaction) the local diffusion coefficient increases with the concentration of infecteds, in the other system (directed reaction) individuals drift proportional to infection level gradients. For both systems we develop a mean field model. Although one expects that the individual rationale of avoiding an epidemic wave mitigates disease dynamics we find extended parameter regimes in which this rationale actually facilitates epidemic spread. Finally we investigate the dynamics of a fully stochastic system in which the effects prevail but which also show an increased extinction probability of the epidemic as a function of increasing dispersal response.

2:54PM D39.00001 Nonstationary increments and variable diffusion processes in financial markets. JOSEPH L. MCCAULEY, KEVIN E. BASSLER, GEMUNU H. GUNARATNE, University of Houston, U OF H ECONOPHYSICS GROUP COLLABORATION — Fat tailed returns distributions and Hurst exponent scaling for financial markets have been reported for more than a decade. The sliding interval technique used in those analyses implicitly assumes that the increments are stationary, an assumption that generally contradicts the facts that the increments are uncorrelated. We show that the data exhibit nonstationary, uncorrelated increments, implying diffusive dynamics with a variable diffusion coefficient, but there is no evidence for either fat tails or Hurst exponent scaling in daily FX returns.
4:30PM D39.00009 A Model for Nonstationary Market Dynamics with Nontrivial Dynamical Scaling

MIN LIU, KEVIN E. BASSLER, University of Houston — In a recent empirical analysis of the Euro/Dollar exchange rate [Bassler, et al., PNAS 104, 17287 (2007)] it was found that during certain periods of the day the market returns scale with Hurst exponents $H$ that are significantly different from 1/2. In some of these periods it is less than 1/2, while in others it is greater than 1/2. In this talk we will propose a possible origin for this behavior and other stylized market facts, including short time negative autocorrelations of returns, in terms of a nonstationary compound Poisson process with a time-dependent intensity rate function that results from a changing bid-ask spread in the microscopic market. The model correctly describes the dynamic scaling behavior of a simple reaction-diffusion model of a limit-order book. That model, like the Euro/Dollar exchange rate, has nonstationary return increments and a Hurst exponent $H$ not equal to 1/2.

4:42PM D39.00010 path integral approach to closed form pricing formulas in the Heston framework

DAMIAAN LEMMENS, MICHEL WOUTERS, JACQUES TEMPERE, Universiteit Antwerpen, SVEN FOULON, KBC Bank, TFVS TEAM — We present a path integral approach for finding closed form formulas for option prices in the framework of the Heston model. The first model for determining option prices was the Black-Scholes model, which assumed that the logreturn followed a Wiener process with a given drift and constant volatility. To provide a realistic description of the market, the Black-Scholes results must be extended to include stochastic volatility. This is achieved by the Heston model, which assumes that the volatility follows a mean reverting square root process. Current applications of the Heston model are hampered by the unavailability of fast numerical methods, due to a lack of closed-form formulae. Therefore the search for closed form solutions is an essential step before the qualitatively better stochastic volatility models will be used in practice. To attain this goal we outline a simplified path integral approach yielding straightforward results for vanilla Heston options with correlation. Extensions to barrier options and other path-dependent option are discussed, and the new derivation is compared to existing results obtained from alternative path-integral approaches (Dragulescu, Kleinert).

4:54PM D39.00011 Modeling income distribution as a sum of additive and multiplicative stochastic processes

ANAND BANERJEE, VICTOR YAKOVENKO, University of Maryland — We obtained an analytical stationary solution of the Fokker-Planck equation for a stochastic process that is a sum of the additive and multiplicative processes. The stationary probability distribution function smoothly interpolates between an exponential distribution at the low end and a power law at the high end. It may have different applications in physics. Here we apply it to income distribution in a society by modeling income as a stochastic process. We analyze the personal income distribution data in USA from the Internal Revenue Service. Using just three fitting parameters (the average income in the exponential part, the power-law exponent, and the crossover point between the exponential and the power laws), we obtain very good fits of the IRS data for a range of years.

5:06PM D39.00012 Power-law behavior and condensation phenomena in disordered urn models: Analysis and its application to macro-economics

JUN-ICHI INOUE, Hokkaido University, JUN OHKUBO, Institute for Solid State Physics, University of Tokyo — We investigate equilibrium statistical properties of a disordered urn model. New types of urn models are proposed, in which quenched disorder parameters play an important role in generating power-law behavior. By choosing an arbitrary energy function for each urn, one can construct a lot of urn models, and we assume that the energy function contains a disordered parameters. We evaluate the occupation probability $P(k)$ that an arbitrary urn has $k$ balls by using the concept of statistical physics of disordered systems. In our new disordered urn model, we find that above critical density $p_c$ for a given temperature, condensation phenomenon occurs and most of the balls are condensed into an urn with the lowest energy level. As the result, the occupation probability changes its scaling behavior from an exponential-law to a heavy tailed power-law in large $k$ regime. We also discuss an application of our results for explaining of macro economy, in particular, emergence of wealth differentials.

5:18PM D39.00013 The Macro Model of the Inequality Process and the Surging Relative Frequency of Large Wage Incomes

JOHN ANGLE, Inequality Process Institute, Maryland, USA — Particles are randomly paired in the Inequality Process (IP), a particle system scattering a positive quantity, wealth. Each particle has a parameter, $\omega$, the fraction of wealth lost in a loss whose probability is 0.5. The stationary distribution of the wealth of particles with $\omega_P$ is approximated by a $\Gamma$ pdf, the IP’s macro model, with shape and scale parameters expressed in terms of $\omega_P$. The model’s dynamics are driven by the product, $\omega_P\mu_t$, where $\omega_P$ is the harmonic mean of the $\omega$’s in the population at time $t$ and $\mu_t$, the population mean of wealth at time $t$. This $\Gamma$ pdf model fits the annual distribution of annual wage income in the U.S. 1961-2003. These data also confirm that the time-series of scalar statistics of wage income that labor economists think are produced by the U.S. distribution of wage income being “hollowed out” (bimodal), the increasing dispersion of wage income and the surging relative frequency of large wage incomes, are produced by the distribution being stretched over larger wage incomes, as implied by the IP’s macro model when $\omega_P\mu_t$ increases. The IP’s macro model includes wage income distribution dynamics into statistical mechanics. To appear in The Econophysics of Markets and Business Networks.

Monday, March 10, 2008 2:30PM - 5:30PM –
Session D40 SPS DBP: SPS Undergraduate Research and Outreach II Morial Convention Center 232

2:30PM D40.00001 Oxide Reliability of SiC MOSFETs

ENRIQUE CARRION, Student, MOSHE GURFINKEL, JOHN SUEHLE — SiC is one of the materials that presents the most promise for harsh environment electronics. Its ability to operate under high temperature and high power, as well as under radiation, made it the material of choice for this study. SiC MOSFETs constitute an important step towards the development of the next generation of resistant electronics. The eventual industrial manufacturing of this type of field effect transistor depends on the effectiveness to improve its performance. Currently, a sudden current degradation, and an unsatisfactory low mobility are observed during the operation of these devices. In this work, we studied both of these drawbacks as a function of temperature. The devices used were SiC nMOSFETs with a SiO$_2$ oxide. Two types of measurements (ultra fast and conventional) were performed during this experience in order to observe 8 decades of current degradation. From our experience, it was observed that as the temperature was lowered the threshold voltage ($V_{TH}$) increased, while the mobility and the drain current ($I_D$) decreased.

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1This study was financially supported by Grant-in-Aid Scientific Research on Priority Areas “Deepening and Expansion of Statistical Mechanical Informatics (DEX-SMI)” of The Ministry of Education, Culture, Sports, Science and Technology (MEXT) No.18079001.

2National Institute of Standards and Technology
2:42PM D40.00002 X-ray degradation studies of Nafion in a PEM fuel cell. REBECCA JENKINS, JUAN FRAGOSO — The overall goal of this research is to test for degradation of the Polymer Electrolyte Membrane (PEM) fuel cells due to exposure to ionizing radiation. We have successfully developed a Membrane Electrode Assembly (MEA) that can be fully disassembled down to the bare Proton Exchange Membrane (PEM) and reassembled repeatedly. This is crucial for testing the degradation effects on the individual components of the MEA. It was also important to establish baseline repeatability of the polarization curves of the MEAs. Therefore, we systematically varied different parameters to test their effect as well as to establish consistent experimental procedures. Hydration of the fuel cell has been found to be crucial for repeatable results. These polarization curves should also have voltages that ranged from 500 V to 1.0 V and current densities up to 11 mA/cm². The Nafion can then be exposed to an x-ray source and the respective polarization data can be studied. A working fuel cell has also been built that fits into the microwave cavity of an electron paramagnetic resonance spectrometer. This allows for the study of behavior of freely radicals formed in a normal operational fuel cell as well as fuel cells with x-ray exposed membranes.

2:54PM D40.00003 Polymer Nanocomposite Gyroids1. CHRIS KNOROWSKI, Virginia Tech, JOSHUA ANDERSON, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Self-assembled polymer phases are increasingly being used in the development of nanocomposite materials. The polymer matrix provides a template for nanoparticles added to the system, transferring the structure of the polymer to the nanoparticles. We perform Molecular Dynamics simulations of these polymer nanocomposite materials and characterize their phase diagrams. Two striking results are found. First, a specific interaction of the polymer and the nanoparticles is required for a successful templating. Second, the presence of nanoparticles can change the pure polymer phase entirely. For instance, a small nanoparticle concentration turns a polymer system from a hexagonal phase into a gyroid phase, both for the polymers and the nanoparticles. In fact, the gyroid is the most prevalent phase over a wide range of interaction strengths and polymer composition.

3:06PM D40.00004 Sol-gel synthesis and characterization of terbium doped tin-oxide1. REBECCA SOBEL, CHRISTIE LAROCHELLE, Franklin and Marshall College — Rare earth doped tin oxide nanocrystals emit visible light when excited in the ultra-violet. Using a sol-gel process, we embedded Tb³⁺ doped SnO₂ nanocrystals in silica glass and characterized the samples using x-ray diffraction, photoexcitation and emission spectroscopy, and transmission electron microscopy. We synthesized four sets of samples, SnO₂:995SiO₂, 35SnO₂:975SiO₂, 55SnO₂:955SiO₂, 75SnO₂:935SiO₂ with constant weight ratios of Tb³⁺ to measure the effects of varying the molar concentrations of Tin-Oxide on the photoluminescence properties of the nanocrystals.

3:18PM D40.00005 Generation of 279nm Light for Single Photon Ionization of Laser Cooled Rubidium. LUCAS WILLIS, MICHAEL LIM, Rowan University — The ionization of rubidium for the formation of ultracold plasma is often done by the nanocrystals.

3:30PM D40.00006 Bio-Photonic Detection of Various Cellular Cultures. PATRICK HANN, MARIA GARZON, ERIK PFEIFFER, SAMUEL LOFLAND, ERNST KNOESEL, Rowan University — Since it is non-invasive, there has been increased research in the field of research addresses some of the challenges associated with growing epitaxial thin films of the CMR manganite material, Nd(SC) grown on substrates Al₂O₃, MgO and seed layers of VC, and TiC at room temperature up to 850°C. HETTINGER, SAMUEL LOFLAND, Rowan University, TED SCABAROZI, Drexel University — We have synthesized and characterized Cr₂AlC thin films with such schemes in place, there exists a mismatch between the thermal expansion coefficients of Silicon (αSi=2.618×10⁻⁶K⁻¹ at 300K) and NSMO (αNSMO =3×10⁻⁶ K⁻¹). This large mismatch induces thermal stresses that deteriorate the film properties. Our research investigates how the thermal stress evolves as a function of the thickness of the multi-layers, and how the process parameters such as the film growth kinetics and thermal kinetics can be optimized to minimize the stress. We are using the Pulsed Laser Deposition technique for thin film growth and characterizing the properties of the sensor layer using X-ray diffraction, electrical resistance measurements, optical microscopy and atomic force microscopy. Acknowledgement: We acknowledge support for this research from Lawrence Livermore National Laboratory.

3:42PM D40.00007 Epitaxial Thin Film Growth of CMR Manganites on Silicon: The Effect of Thermal Stress. SANJAY ADHIKARI, BAO HA, GRACE YONG, DAVID SCHEFER, RAJESWARI KOLAGANI, Towson University — Our algae will be presented and compared to other reports in the literature and procedure for the detection of these ultra-weak photonic emissions using a single photon detection device. The results of bread yeast, saccramyces, and

3:54PM D40.00008 Synthesis and Characterization of Cr₂AlC Thin Films. JUAN ROCHE, JEFFREY HETTINGER, SAMUEL LOFLAND, Rowan University, TED SCABAROZI, Drexel University — We have synthesized and characterized Cr₂AlC thin films grown on substrates Al₂O₃, MgO and seed layers of VC, and TiC at room temperature up to 850°C. Texture films were successfully grown above 550°C while Raman spectroscopy shows vibrations down to 500°C. Films below 500°C down to room temperature show texturing upon annealing at 750°C. The films were prepared using RF magnetron sputtering from elemental targets. Electrical transport shows metallic behavior of the films down to 10 K. EDS was used to verify chemistry from which the MA ratios were found that a slight deviation still allowed formation of the MAX phase. X-ray diffraction shows that when the chemistry is off it results in secondary phases of Cr₂6C₆ and Cr₂Al. Atomic Force Microscopy (AFM) shows smoother films at lower temperatures and rougher films at higher temperatures with a surface roughness > 20 nm. Friction test results will be presented.

4:06PM D40.00009 Spatially resolved quasi-particle tunneling spectra in the vortex state of optimally hole-doped YBa₂Cu₃Oₓ (Y-123). M.S. GRINOLDS, A.D. BEYER, M.L. TEAGUE, N.-C. YEH, Phys. Dept., Caltech, Pasadena, CA — We report cryogenic scanning tunneling spectroscopic (STS) studies of superconducting single crystalline Y-123 (Tc = 93 K) as a function of magnetic field. We study and model the influence of competing orders (COs), which coexist with superconductivity (SC), on the quasiparticle (QP) excitation spectra. The spatial dependence of the QP tunneling spectra is probed via STS to quantify the presence and spatial extent of SC and CO. Zero-field spatial maps of the QP spectra (100×100 nm²) in Y-123 exhibit long-range spatial homogeneity of SC (ΔSC = 23±1 meV) associated with the spectral coherence peaks and the presence of CO (ΔCO = 33±2 meV) that gives rise to the spectral satellite features at ΔCOeff = [2(DCO)² + (VCO)²]¹/². Conductance maps of the Y-123 in finite fields demonstrate spatially varying spectra consistent with the periodicity a₀ of the vortex lattice, with pseudogap (PG) like features at ΔCOeff inside the vortex core and SC gap features remaining at ∼ΔSC outside the vortex core. Moreover, conductance histograms of the vortex state reveal that the ratio of the areas associated with ΔSC and VCO is comparable to (a₀/ξab)², (ξab: in-plane SC coherence length). These results therefore suggest the important role of COs in the cuprate QP excitations. This work is supported by NSF Grant DMR-0405088.
4:18PM D40.00010 High Frequency Electrical Properties of Carbon Nanotubes

DOBROMIR KAMBUROV, BETH PARKS, Colgate University, ZHAOHUI ZHONG, PAUL MCEUEN, Cornell University — We report on measurements of the high frequency electrical properties of single-walled carbon nanotubes. These measurements are accomplished by incorporating a single nanotube into a microwave stripline and using optical pulses from a femtosecond laser to create short electrical pulses on the stripline. By varying the time delay between the pulses, it is possible to determine the frequency dependence of the response of the nanotube.

This work was supported by the NSF through the Center for Nanoscale Systems. Sample fabrication was performed at the Cornell Nanoscale Science and Technology Facility, a National Nanotechnology Infrastructure Network node, funded by NSF.

4:30PM D40.00011 Current State of Research of Alternate Fuel Sources for Passenger Vehicles

LEE MASSEY, University of Wisconsin at River Falls — The purpose of this project is to report on the current state of research in the field of alternate fuel sources for passenger vehicles. Because the number of alternate fuel options is very large, this study focuses on selected bio-fuels and briefly describes a couple of the most popular non-bio and non-renewable alternatives. The fuel and energy sources studied are compared using well-to-wheel and well-to-tank net energy balances. Data also includes relative production capabilities by volume in terms of current fossil fuels. Qualitative data includes production methods and transportability.

Research funded by APS Fellowship in the Forum on Physics and Society.

4:42PM D40.00012 Universal Properties of Population Dynamics with Fluctuating Resources

SAIYAK MUKHERJEE, Virginia Tech, HANS-KARL JANSEN, Heinrich-Heine-Universitat, Dusseldorf, BEATE SCHMITTMANN, Virginia Tech — Starting from the well-known field theory for directed percolation, we describe an evolving population, near extinction, in an environment with its own nontrivial spatio-temporal dynamics. Here, we consider the special case where the environment follows a simple relaxational (Model A) dynamics. Two new operators emerge, with upper critical dimension of four, which couple the two theories in a nontrivial way. While the Wilson-Fisher fixed point remains completely unaffected, a mismatch of time scales destabilizes the usual DP fixed point, suggesting a crossover to a first order transition from the active (surviving) to the inactive (extinct) state.

4:54PM D40.00013 First-principles density-functional theory investigation of FOX-7

BRIAN VOHASKA, MICHAEL CONROY, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — Due to the expense and difficulty of experimental investigation of the chemical and physical properties of energetic materials (EMs), computational methods provide a unique opportunity for accurate determination of the chemical and physical properties of EM molecular crystals based on underlying atomic structure. In this presentation, we discuss the results of first-principles density functional theory (DFT) calculations of hydrostatic and uniaxial compression of the important energetic material, FOX-7. The calculated equilibrium properties, such as lattice parameters, elastic constants, and bulk modulus will be reported and compared with experiment, as well as the isothermal equation of state. Due to the anisotropic nature of energetic molecular crystals, physical properties such as cohesive energy, band gap, and stress-strain relationships are reported as functions of uniaxial compression studied. In addition, the shear stress behavior upon uniaxial compression will be discussed, as well as its possible relation to anisotropic shock-sensitivity in FOX-7.

5:06PM D40.00014 Variational Wavefunction Monte Carlo method applied to electrons in a two dimensional square lattice with zero doping

SUNITA KANNAN, COURTNEY LANNERT, Wellesley College — We present the theoretical results from the Variational Wavefunction Monte Carlo method applied to electrons in cuprates, of a two dimensional square lattice with zero doping. Since the true Hamiltonian of the cuprates is not definitively known, much study has gone into identifying the best possible Hamiltonian. To do this, we vary the terms in the Extended Heisenberg Hamiltonian - the neighbor spin coupling term J, the spin next-neighbor term J' and the spin ring exchange term Jring, where each variable represents a different electronic interaction. We then use the variational approach to find the best groundstate wavefunction for each Hamiltonian. Once we find the best groundstate wavefunction for each Hamiltonian, we can deduce the magnetization predicted by that model. Hence, by comparing our results for the magnetization to known experimental results, we can identify the most suitable model.

5:18PM D40.00015 Quantum Criticality and Neutron Scattering Solutions for a Spin-1/2 Ladder Model

JUSTIN COHEN, JEREMIAH BARRY, MARK MEISEL, University of Florida — Exact solutions for a two dimensional, S = 1/2 quantum spin ladder model are obtained through mapping the Hamiltonian and correlation functions onto those of a one dimensional Ising chain model [1]. These solutions include a three dimensional ground state phase diagram, establishing states of ladder rung singlets, triplets, and alternating singlets and triplets in terms of interaction parameters and applied magnetic field. Evidence of quantum criticality is uncovered for select regions of the phase diagram through explorations into ladder site correlations and correlation lengths. Neutron scattering solutions for scattering intensities provide insight into the energy spectra associated with various rung spin configurations.


This work was supported, in part, by the National Science Foundation via DMR-0701400 and grants for the NHMFL and UF Physics REU Summer 2007 Programs.

Monday, March 10, 2008 8:00PM - 9:30PM —
Session G1 APS: 25 Years of Scanning Probe Microscopy New Orleans Marriott Carondelet (3rd floor)

8:00PM G1.00001 Classical Computation in Quantum Nanostructures: A Long Road to an Uncertain Future

DONALD EIGLER, IBM Almaden Research Center — We have extended the spectroscopic abilities of the scanning tunneling microscope to include the measurement of spin-excitation spectra, making it possible to measure the g-value of single atoms. Utilizing spin-excitation spectroscopy as our primary tool, we are now capable of extracting exchange coupling energies, anisotropy energies, and information on the ground and excited state spin configurations of nanometer-scale structures. These experiments are playing an integral role in our efforts to engineer the "energy landscape" of a system of spins in order to achieve nanometer-scale binary logic circuits that operate using only the spin degree of freedom.

Work done in collaboration with Cyrus Hirjibehedin, Andreas Heinrich, Christopher Lutz, Jay Gupta, and Bruce Melior.
Magnetic Exchange Force Microscopy (MExFM), offers a powerful new tool to investigate different types of spin-spin interactions based on direct-, super-, or RKKY-type exchange down to the atomic level. By combining MExFM with high-precision measurements of damping forces, localized or confined spin excitations in magnetic systems of reduced dimensions now become experimentally accessible. Moreover, the combination of spin state read-out and spin state manipulation, based on spin-current induced switching across a vacuum gap by means of SP-STM [9], provides a fascinating novel type of approach towards ultra-high density magnetic recording without the use of magnetic stray fields.

Hole-Mediated Interactions

This work was supported by the ONR MURI program. In collaboration with M. H. Mikkelsen, J.-M. Tang, M. E. Flatté, A. C. Gossard, and D. D. Awschalom.

8:36AM H1.00002 Atom-by-Atom Substitution of Mn in GaAs and Visualization of their Hole-Mediated Interactions, ALI YAZDANI, Princeton Univ — No abstract available.

9:12AM H1.00003 Zero-field optical manipulation of magnetic ions in semiconductors1, ROBERTO C. MYERS2, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — For coherent spin information processing, spin coherence times must be long enough to perform multiple state operations, thus requiring a balance between gating time and spin lifetime. Because single magnetic spins in semiconductors can be strongly coupled to both itinerant carriers and to other magnetic ions, these interactions can be rapidly manipulated optically and electrically. We show that small numbers of magnetic spins in III-V GaAs quantum wells can be polarized by optical spin injection without the need for applied magnetic fields, and exhibit unusually long coherence times: Nm ions provide acceptor states within the bandgap of GaAs enabling optical readout and control of the magnetic ions in a manner distinct from paramagnetic II-VI materials. Spin polarized electrons created within the quantum well dynamically orient the Mn spins in a manner analogous to dynamic nuclear polarization, generating a dynamic exchange splitting of the magnetic spins. The Mn ions’ magnetic moments can be flipped from +1 to -1 by optical excitation and optical power densities as low as 100 mW/mm² are sufficient to invert the population. These results indicate that hole-mediated Mn-Mn interactions dominate the decoherence, and suggest that long lifetimes may be expected for single Mn spins in GaAs.

1This work was supported by the ONR MURI program.

9:12AM H1.00003 Zero-field optical manipulation of magnetic ions in semiconductors1, ROBERTO C. MYERS2, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — For coherent spin information processing, spin coherence times must be long enough to perform multiple state operations, thus requiring a balance between gating time and spin lifetime. Because single magnetic spins in semiconductors can be strongly coupled to both itinerant carriers and to other magnetic ions, these interactions can be rapidly manipulated optically and electrically. We show that small numbers of magnetic spins in III-V GaAs quantum wells can be polarized by optical spin injection without the need for applied magnetic fields, and exhibit unusually long coherence times: Nm ions provide acceptor states within the bandgap of GaAs enabling optical readout and control of the magnetic ions in a manner distinct from paramagnetic II-VI materials. Spin polarized electrons created within the quantum well dynamically orient the Mn spins in a manner analogous to dynamic nuclear polarization, generating a dynamic exchange splitting of the magnetic spins. The Mn ions’ magnetic moments can be flipped from +1 to -1 by optical excitation and optical power densities as low as 100 mW/mm² are sufficient to invert the population. These results indicate that hole-mediated Mn-Mn interactions dominate the decoherence, and suggest that long lifetimes may be expected for single Mn spins in GaAs.
8:36AM H2.00002 From high Tc superconductivity to quantum spin liquids, PATRICK A. LEE, MIT

The underdoped cuprates exhibit many unusual properties going under the name pseudogap. These observations lend support to the notion that high Tc superconductivity is intimately tied to doping of a Mott insulator. Building on earlier work on the quantum spin liquid, the resonating valence bond (RVB) idea of Anderson provides an adequate physical understanding of the pseudogap. The problem can be formulated as a gauge theory even though many details are beyond the powers of current calculational tools. Part of the difficulty is that the pseudogap phenomenology occurs only at finite temperature where precise statements about excitations and possible emergent gauge fields cannot be made. Meanwhile the problem of the quantum spin liquid is a simpler version of the high Tc problem where significant progress has been made recently. It is understood that the existence of a matter field can lead to deconfinement of the U(1) gauge theory, and novel new particles such as fermionic spinons which carry spin 1/2 and no charge, and gapless gauge bosons can emerge in a new critical state at low temperatures. Two experimental systems, the organic compound and the Kagome lattice, have emerged as promising examples of a spin liquid. I shall argue that these may be described by a spinn Fermi surface and Dirac spinons coupled to a U(1) gauge field, respectively. Further experimental tests will be discussed.

References:


— 9:12AM H2.00003 On the pseudogap in high temperature superconductors, ANDREW MILLIS, Department of Physics, Columbia University — The “pseudogap,” a suppression of the density of states observed in at least some high temperature copper-oxide superconductors at carrier concentrations lower than that which maximizes the superconducting transition temperature, presents a long-standing and still unresolved problem in condensed matter physics. Basic questions including whether it is a signature of a new phase of matter or a consequence of thermal or quantal disordering of a superconducting or spin density wave state, remain unresolved. This talk will summarize the present status of the problem, including what is known about the form of the low temperature gap function (one gap or two), the role of thermal scattering in the formation of “fermi arcs” and the significance of recent recent high-field quantum oscillation experiments.

References:


— Second round of contributed talks: 9:48AM H2.00004 Superconductivity, quasi-particle dynamics and strong-coupling physics, JOERG SCHMALIAN, Ames Laboratory, Iowa State University — I discuss the problem of superconductivity from the perspective of pairing mediated by a boson and compare with the situation of “no-glue” superconductivity in a strongly correlated material. This is done for Ti-doped PbTe, where recent experiments support superconductivity due to quantum valence (charge Kondo) fluctuations, and for the doped Mott insulator SrCu2(BO3)2, where d-wave superconductivity emerges due to a reorganization of a valence bond crystal state. I discuss the implications of these results for high temperature superconductivity in the cuprates.

1. Support from NSF-DMR 0705874.

Tuesday, March 11, 2008 8:00AM - 11:00AM
Session H3 DPOLY: Polymer Physics Prize Morial Convention Center RO2 - RO3

8:00AM H3.00001 Polymer Prize Talk: Segmental Dynamics in Polymers: From Cold Melts to Aging and Stressed Glasses, STEVEN KIVELSON, Stanford

In the cold molten state they exhibit chemically-specific and strongly non-Arrhenius segmental relaxation which sets the time scale for the generic chain scale dynamics. In the amorphous solid or plastic state the temperature dependence of the alpha relaxation time changes, physical aging emerges, and a rich mechanical response occurs characterized by the dynamic yielding, strain softening and strain hardening processes. We have developed a statistical mechanical theory of activated segmental relaxation in cold melts by combining and extending methods of mode coupling, dynamic density functional and activated hopping theories. The approach is built on the concept of a confining nonequilibrium free energy which quantifies local dynamical constraints and the barrier hopping process. The localizing consequences of interchain caging forces are quantified by the amplitude of nanometer scale density fluctuations (compressibility) and backbone stiffness. Predictions for the kinetic glass and dynamic crossover temperatures, dynamic fragility, and thermal dependence of the segmental relaxation time are consistent with experiments. The theory has been generalized to treat alpha relaxation, physical aging, and nonlinear mechanical properties in the glass. The structural component of density fluctuations become (partially) frozen resulting in a crossover to Arrenhius relaxation. Physical aging is modeled based on a kinetic equation for collective density fluctuations. At intermediate time scales the relaxation time (shear modulus) grows as a power law (logarithmic) function of aging time with a temperature dependent exponent. Applied stress weakens dynamical constraints thereby accelerating relaxation and softening the elastic modulus. A constitutive equation has been constructed from which the temperature dependent dynamic yielding and mechanical response under constant strain rate, constant stress (creep), and other modes of deformation can be calculated. This work was done in collaboration with Drs. Kang Chen and Erica J. Saltzman.
and Simon Abay

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and scanning tunneling probes. The change in dissipation of the device will translate into a magnitude change of the reflected signal. Non-dissipative devices
and non dissipative nanodevices can be measured in this way. Typical examples of dissipative devices are single electron transistors, quantum point contacts
with resonant circuits using rf and microwave techniques. We will review a number of nanodevices probed with rf and microwave methods, both dissipative
and non dissipative nanodevices. Such devices can be extremely sensitive sensors, but they typically operate at low temperatures and have high impedances.
These studies are motivated by a desire to understand properties of polymer nanocomposites where the role of particle/polymer segment interactions is
poorly understood but the state of particle dispersion is key to composite properties. In this talk I explore equilibrium and nonequilibrium phases of this system
and compare with extant theoretical approaches.

9:12AM H3.00003 Complex Fluid Microstructure, Rheology and Glass Transitions: Effect of Continuous Phase Molecular Weight , CHARLES ZUKOSKI, University of Illinois — The mechanical properties of suspensions depend dramatically on the suspension microstructure. Microstructure in turn depends on the nature of particle interaction potentials. For those systems that are thermodinamically activated there will be an equilibrium microstructure and thus equilibrium transport properties. One of the model systems used to understand the links between interactions, microstructure and transport properties is that of hard spheres suspended in a Newtonian continuous phase. This model system can be studied experimentally and direct comparisons made with model predictions. With the increase in particle volume fraction, if the particles cannot crystallize, the suspension forms a glass where long range self diffusion is essentially eliminated. The approach to the glass transition has been studied experimentally and agreement with models is strong. In this talk we discuss what changes as the continuous phase takes on a granularity where the continuous phase molecules have substantial degrees of freedom. In particular, we investigate the mechanics and microstructure of hard sphere suspensions in polymer melts. The particles are composed of silica while we use polyethelene glycols of different weights ranging from small degrees of polymerization through the entanglement molecular weight. These studies are motivated by a desire to understand properties of polymer nanocomposites where the role of particle/polymer segment interactions is poorly understood but the state of particle dispersion is key to composite properties. In this talk I explore equilibrium and nonequilibrium phases of this system and compare with extant theoretical approaches.

9:48AM H3.00004 Dynamics of fluids in complex environments , ARUN YETHIRAJ, University of Wisconsin — No abstract available.

10:24AM H3.00005 The Theta Point Of Long Flexible Polymer Chains: When Does It Exist?1 , K. BINDER, Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — The standard description of the conformation of a long flexible polymer coil in dilute solution implies a swollen state under good solvent conditions, while deterioration of solvent quality (by decrease of temperature) causes a (gradual) chain collapse below the Theta point. At the Theta point, the chain follows Gaussian statistics, apart from logarithmic corrections. Monte Carlo simulations of the bond fluctuation model will be discussed that provide evidence for a second scenario, where the chain experiences a first order transition from the swollen state to a dense solid phase, provided the range of effective attractive interactions is sufficiently short. This scenario then implies that in solution at finite concentration no vapor-liquid-like phase separation occurs. The analogy between this prediction and the behavior of some colloidal dispersions is discussed.

1In collaboration with W. Paul, F. Rampf, and T. Strauch.

Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H4 DMP: Selected Applications Using Materials Science Morial Convention Center 206

8:00AM H4.00001 Integrated Functionality: Nanosensors , JOZEF T. DEVREESE, Theoretical Physics of the Solid State (TFVS), Universiteit Antwerpen, Belgium — Integrated nanosensors are nanostructured systems in which several sensors of different types have been integrated on a single platform including those sensitive to optical, magnetic, chemical, or biological stimuli [1,2]. Nanoparticle-based detector systems rely on the development of nanoparticles as sensing species. I discuss state-of-the-art nanosensors which are based on various advanced materials: nanoshells and nanorice, gold nanoparticles with attached fluorescent dyes, nanopores, carbon nanotubes, neuroelectronic hybrid systems, semiconductor nanocrystals and quantum-dot quantum wells (QDQW’s). Phonon-assisted optical processes in semiconductor nanocrystals and QDQW’s are highly sensitive to their shape and geometry i. a. due to the non-adibaticity of the exciton-phonon systems. This sensitivity opens new perspectives for applications of quantum dots in optical sensing. For example, the simultaneous consideration of the tetrahedral shape of a CdS/HgS/CdS QDQW, interface optical phonons, and non-adibatic phonon-assisted transitions allows for control of the photoluminescence of a QDQW [3]. Quantum-dot-based systems are also considered as examples of communication with nanodevices, which is a prerequisite of their integration. Nanosensors allow for building a new class of integrated devices, which provide the elemental base for “intelligent sensors” capable of data processing, storage and analysis. The development of integrated nanosensors could have many applications in several fields such as process monitoring, robotics, environmental, medical, consumer, homeland security... [1] I. K. Schuller, http://nanosensors.ucsd.edu/Introduction.htm. [2] J. T. Devreese and Y. Bruynseraede, Integrated Nanosensors. McGraw-Hill 2008 Yearbook of Science & Technology, McGraw-Hill, 2008. [3] V. A. Fonoberov, E. P. Pokatilov, V. M. Fomin, and J. T. Devreese, Phys. Rev. Lett. 92, 127402 (2004).

8:36AM H4.00002 ABSTRACT WITHDRAWN —

9:12AM H4.00003 Nanodevice sensors measured with rf- and microwave reflectometry1 , PER DELSING, Chalmers University of Technology — Nanodevices can be extremely sensitive sensors, but they typically operate at low temperatures and have high impedances. This makes it hard to measure these devices at high frequencies, however this problem can be overcome by impedance matching these devices with resonant circuits using rf and microwave techniques. We will review a number of nanodevices probed with rf and microwave methods, both dissipative and non dissipative nanodevices can be measured in this way. Typical examples of dissipative devices are single electron transistors, quantum point contacts and scanning tunneling probes. The change in dissipation of the device will translate into a magnitude change of the reflected signal. Non-dissipative devices like parametric capacitances or inductances of superconducting circuits give rise to a shift in the resonance frequency of the resonant circuits which results in a phase shift of the reflected signal. Using these methods drastically increases the operation frequency and often also the sensitivity of the measured quantity. The non dissipative devices also have very low back-action and can potentially approach the limits set by quantum mechanics.

1Work in collaboration with Christopher Wilson, Timothy Duty, Jonas Bylander, Sergey Kafanov, Martin Sandberg, Fredrik Persson, Martin Gustavsson, and Simon Abay.
Materials Informatics: Using machine learning techniques with large amounts of ab-initio computed or experimental data, GERBRAND CEDER, Massachusetts Institute of Technology — Machine learning techniques can be applied to large amounts of experimental or computed materials data in order to identify the underlying factors that determine a target property. While the use of experimental data is complicated by the fact that it is mostly non-standardized in property or structure databases, experimental data still tends to be richer in information than computed data. One problem that can be addressed with machine learning techniques is the prediction of structure. By using structure prototype as a mathematical descriptor, and constructing its correlation in chemical spaces through machine learning techniques, it is possible to create a highly effective structure prediction method. Previously, we demonstrated that by simply applying maximum entropy ideas to a large experimental structure database of binary metals, it was possible to suggest a short list of candidate structures for new compounds which contains the proper ground state with very high probability [Ref]. This list of probable structures can then be computed with ab initio energy methods. We have now extended this method to multi-component and non-metal systems by prototyping the ≈ 100,000 structure records in the International Crystallographic Structure Database, and a similar accuracy of prediction is achieved in these high component spaces. We believe that such a machine learning approach solves the crystal structure prediction for many practical purposes. Machine learning techniques can also be used to point at likely errors in experimental structure databases and I will give some examples. In the long-term computed data is more likely to form the input for machine learning techniques as it is well defined and obtained under controlled conditions. Using high-throughput ab-initio computing techniques we have determined the structure and energy for several thousand compounds and have begun to data mine this information for property models relevant to energy generation and storage.

Tuesday, March 11, 2008 8:00AM - 10:24AM – Session H5 DCMP: CeMn5 (115) Heavy Electron Materials: A Rosetta Stone for the Kondo Lattice? Morial Convention Center R01

8:00AM H5.00001 Angle-resolved Photoemission of CeCoIn₅: Detailed Comparison to LDA and LDA+DMFT, J.W. ALLEN, University of Michigan — Highly-activated photon-dependent angle resolved photoemission spectroscopy (ARPES) in the energy range of 80-200 eV has been used to characterize the three dimensional (3D) Fermi surface (FS) topology and electronic band structure of cleaved single crystals of CeCoIn₅. The sample temperature of ≈ 20K is well below the lattice coherence onset temperature at ≈ 45K found in a recent "two fluid" analysis of transport data. Detailed comparison of ARPES FS contours to LDA calculations for the Ce 4f electrons treated as itinerant or confined to the core reveals remarkable agreement to fine topological details of the f-core calculations. Also in agreement to the f-core calculations is the experimental absence of extra electron-like contours predicted in the f-itinerant calculation, originating from α and β bands re-enterant below E_F along Z-A. Finally, the areas enclosed by FS contours for the α and β bands are significantly smaller than are found in very low temperature CeCoIn₅ de Haas van Alphen data that agrees generally with the f-itinerant calculation. It is concluded that clear signatures of coherence in the transport data can develop at temperatures for which the f-electrons are not yet included in the FS. In this connection, comparison will also be made to recent DFT-LDA+DMFT calculations for CeIrIn₅. This work was done in collaboration with J. D. Denlinger, Peng Wang, R. S. Singh, K. Rossnagel, S. Elgazzar, P. M. Oppeneer, V. S. Zapf and M. B. Maple. and was supported by the U.S. DOE (DE-AC02-98CH10886 and the ALS) and NSF (DMR-04046105 at UCSD), by the U.S. NSF (DMR-03-02825 at UM for initial work, DMR-03-35173 at UCSD) and by the Swedish Research Council (VR) and the European Commission (JRC-ITU).

8:36AM H5.00002 Modeling the Localized to Itinerant Electronic Transition in the Heavy Fermion System CeIrIn₅, KRISTJAN HAULE, Rutgers University — Within the ab-initiation calculation we adress the crossover from localized itinerant state of a heavy fermion material CeIrIn₅. The temperature evolution of the one electron spectra and the optical conductivity is predicted from first principles. The buildup of coherence in the form of a dispersive many body feature is followed in detail and its effects on the conduction electrons of the material is revealed. We find multiple hybridization gaps and link them to the crystal structure of the material. Our theoretical approach explains the multiple peak structures observed in optical experiments and the sensitivity of CeIrIn₅ to substitutions of the transition metal element and may provide a microscopic basis for the more phenomenological descriptions currently used to interpret experiments in heavy fermion systems.

9:12AM H5.00003 Andreev reflection in heavy fermions and the superconducting order parameter in CeCoIn₅, WAN KYU PARK, Department of Physics and the Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — Andreev reflection, a retro-reflection of an incoming electron as a hole at a normal-metal/superconductor interface, is well understood in conventional superconductors. However, Andreev reflection in heavy-fermion superconductors, the microscopic consequences of the heavy electronic mass remain an open question. According to the Blonder-Tinkham-Klapwijk (BTK) theory, no Andreev process is allowed because of the large mismatch in the Fermi velocities [1]. However, conductance enhancement due to Andreev reflection, albeit reduced, has been frequently observed in heavy-fermion superconductors [2]. In this talk, I will present such conductance spectra obtained along three different crystallographic orientations of the heavy-fermion superconductor CeCoIn₅ [3]. Qualitative analysis using the extended BTK model shows the first spectroscopic evidence for dₓ²−ᵧ²-wave (instead of dₓᵧ-wave) symmetry, resolving the controversy over the node locations. In order to explain the reduced Andreev signal and the conductance asymmetry, both commonly observed in heavy-fermion superconductors, we propose a conductance model based on the two-fluid phenomenology [4] and an assumed energy-dependent density of states. I will discuss the significance of this model and possible clues for developing it into a microscopic theory. [1] G. E. Blonder, M. Tinkham, and T. M. Klapwijk, Phys. Rev. B 25, 4515 (1982); [2] G. E. Blonder and M. Tinkham, Phys. Rev. B 27, 112 (1983); [3] Y. G. Naidyuk and I. K. Yanson, J. Phys.: Condens. Matter 10, 8905 (1998); [4] W. K. Park et al, arXiv:0709.1246 (submitted to Phys. Rev. Lett.).
of passive and active microrheology. Measured the dynamics and mechanical properties of a simple three-component model system, consisting of myosin II, actin filaments, and crosslinkers. Stresses forces using their mechanical framework, the cytoskeleton, which is a non-equilibrium, composite material including polymers and motor proteins. We have, CHRISTOPH SCHMIDT, Georg-August-Universität, Fakultät für Physik, III. Physikalisches Institut — Cells both actively generate and sensitively react to

8:36AM H6.00002 Tornadoes and Severe Thunderstorms: Physical Understanding and Climate Questions, HAROLD BROOKS, National Severe Storms Laboratory — Severe thunderstorms (those that produce large hail, high winds and/or tornadoes) are of importance because of the threat to life and property they pose. This talk will review our understanding of the physical processes that lead to them and their distribution in time and space. The basic approach follows that of weather forecasting, focusing on the atmospheric “ingredients” in the environment necessary to produce severe thunderstorms and tornadoes, particularly the thermodynamic state of the atmosphere and the organizing effects of vertical wind shear that leads to the most severe storms. We will look at the challenges of reconciling our limited reporting databases of events and our physical expectations derived from the distribution of those environmental conditions. Consistent (and inconsistent) aspects of the various databases around the world will be discussed with their implications for what we can and cannot say about the basic physical processes. Of particular interest is the record from the United States. Some simple efforts to deal with the spatial and temporal inhomogeneities in the observational record will be developed with the limits that are implied on our ability to detect past changes. Finally, the talk will close with a discussion of the possible effects of anthropogenic global warming on severe thunderstorms, particularly in the United States. Global climate model studies of this problem are very recent, with the first peer-reviewed results appearing in 2007. The limitations of the climate models and possible scenarios for the future will be discussed.

9:12AM H6.00003 Factors Influencing Hurricane Surges along the Louisiana-Mississippi Coast, DONALD T. RESIO, U.S. Army Engineer Research and Development Center — The effects of recent hurricanes along U.S. Coastlines, along with expected future sea level rise and the potential for increased storm activity all point to a critical need for improved methods for estimating coastal hazards and associated risks. Many of the models used today to assess hazards and risk incorporate considerable empiricism in their formulation. Unfortunately, most of the empirical evidence is drawn from small to moderate storm events and cannot be effectively extrapolated to extreme storms such as Hurricane Katrina. This presentation will critique the state of the art in hurricane surge prediction, including the adequacy of numerical models, coefficients within these models, and the wind fields utilized to force them. Once the predictive system and its physical basis are introduced and discussed, a methodology will be described for utilizing information from such a system to estimate risk for coastal areas, including the effect of uncertainties in both the modeling system and storm climate. Using the methodology introduced here, maps of estimated storm surge levels for selected recurrence intervals in the New Orleans area will be presented along with a comparison to some previously derived values to provide perspective.

9:48AM H6.00004 Wetland Loss and Restoration Options in Southern Louisiana, ROBERT G. DEAN, University of Florida — Wetlands are productive landscape features of the broad Mississippi River Delta system. In addition to their ecological services of providing habitats for a variety of species including juvenile commercial and recreational fish, they provide a valuable wave reduction role during severe storm events characterized by elevated water levels and high waves. Currently, these wetlands are stressed by a combination of natural and human-related forces resulting in rapid loss rates. Although many factors contribute to wetland loss rates, the single greatest factor is the shunting of river borne sediments offshore into deep water. Navigational interests benefit greatly from the present fixed location of the main navigation channel at Southwest pass with its terminus at the edge of the continental shelf such that the sediment load is discharged into deep water. The Mississippi River Delta region is subsiding at up to more than 10 times the Eustatic rate of sea level rise and thus the wetland and barrier island systems require these sediments for maintenance and growth. With the increasing scarcity and costs of energy, it is highly desirable that wetland restoration be done using natural forces to the degree possible. Absent legal issues, a pragmatic approach could be to identify those areas where progress can be made with realistic investments of economic and energy resources and to accept that areas with less benefit per investment will continue to degrade. The paper will review various options and discuss obstacles and opportunities.

Tuesday, March 11, 2008 8:00AM - 11:00AM —

Session H7 DBP DPOLY: Complex Active Biomaterials: Mechanics and Microrheology Morial Convention Center R05

8:00AM H7.00001 Non-equilibrium mechanics of motor-driven cytoskeletal polymer networks, CHRISTOPH SCHMIDT, Georg-August-Universität, Fakultät für Physik, III. Physikalisches Institut — Cells both actively generate and sensitively react to forces using their mechanical framework, the cytoskeleton, which is a non-equilibrium, composite material including polymers and motor proteins. We have measured the dynamics and mechanical properties of a simple three-component model system, consisting of myosin II, actin filaments, and crosslinkers. Stresses arising from motor activity control network mechanics: both increasing stiffness by a factor of nearly 100 and qualitatively changing the viscoelastic response of the network in an ATP-dependent manner. We have quantified the mechanical properties as well as the active fluctuations in these networks by a combination of passive and active microrheology.
8:36AM H7.00002 Non-equilibrium mechanics and dynamics of active gels and living cells. FRED
MACKINTOSH, Vrije Universiteit — Much like the bones in our bodies, the cytoskeleton consisting of filamentous proteins largely determines the mechanical response and stability of cells. Such important cellular processes as locomotion, cell division, and mechanosensing are largely governed by complex networks of cytoskeletal biopolymers and associated proteins that cross-link these and/or generate forces within the network. In addition to their important role in cell mechanics, cytoskeletal biopolymers have also provided new insights and challenges for polymer physics and rheology. In the cell, however, these polymer networks or gels are far from equilibrium in a way unique to biology: they are subject to active internal force generation by molecular motors. We describe recent theoretical and experimental results on active in vitro networks that demonstrate significant stiffening and non-equilibrium fluctuations due to motor activity [1]. We show how this activity leads generically to a colored, 1/ω spectrum of force fluctuations, which can account for surprisingly Brownian-like motion in elastic networks. We also discuss how the fluctuations of individual cytoskeletal filaments can be used to probe both mechanical properties and non-equilibrium activity in living cells [2].


9:12AM H7.00003 Cytoskeletal mechanics: Structure and Dynamics. ANDREAS BAUSCH, Technische
Universität München — The actin cytoskeleton, a dynamic network of semiflexible filaments and associated regulatory proteins, is responsible for the extraordinary viscoelastic properties of cells. Especially for cellular motility the controlled self assembly to defined structures and the dynamic reorganization on different time scales are of outstanding importance. A prominent example for the controlled self assembly are actin bundles: in many cytoskeletal processes cells rely on the tight control of the structural and mechanical properties of the actin bundles. Using an in vitro model system we show that size control relies on a mismatch between the helical structure of individual actin filaments and the packing symmetry within bundles. While such self assembled structure may evoke the picture of a static network the contrary is the case: the cytoskeleton is highly dynamic and a constant remodeling takes place in vivo. Such dynamic reorganization of the cytoskeleton relies on the non-static nature of single actin/ABP bonds. Here, we study the thermal and forced unbinding events of individual ABP in such in vitro networks. The binding kinetics of the transient crosslinkers determines the mechanical response of such networks – in the linear as well as the non-linear regime. These effects are important prerequisites for the high adaptability of cells and at the same time might be the molecular mechanism employed by them for mechanosensing.

9:48AM H7.00004 Micro rheology in Active Cytoskeletal Networks. ALEX LEVINE, UCLA, Department of
Chemistry & Biochemistry — The mechanics of the in vivo cytoskeleton is controlled in part by the details of its non-equilibrium steady-state. In this "active" material, molecular motors (e.g. myosin) exert transient contractile stresses on the F-actin filament network, driving it into a particular non-equilibrium state. Since micro rheology traditionally relies on the linear response properties of the soft materials in thermal equilibrium, this departure from equilibrium has profound implications for the interpretation of rheological properties from the interior of living cells and in vitro active networks. In active networks, such as the in vitro systems of Mizuno et al. [Science 315 (5810) pp. 370-373 (2007)] and in living cells, the underlying theoretical foundation of the interpretation of microrheology – the Fluctuation-Dissipation theorem – does not apply. New ideas are needed. In this talk, I review micro rheology, and then discuss a new theoretical interpretation of microrheology in active (i.e. molecular motor driven) networks. To develop this theory, I introduce a motor-driven, two-fluid model of the active network and background (aqueous) solvent. Using this model and knowledge of the statistical properties of the molecular-motor induced forces, I calculate the non-equilibrium fluctuation spectrum expected for single- and two-particle micro rheology in the driven system. I then compare these results to the data of Mizuno et al..

10:24AM H7.00005 Force fluctuations and polymerization dynamics of intracellular microtubules. CLIFFORD BRANGWYNE, Max Planck Institute — Microtubules are dynamic biopolymers within the cytoskeleton of living cells. They play a central role in many biological processes including cell division, migration, and cargo transport. Microtubules are significantly more rigid than other cytoskeletal biopolymers, such as actin filaments, and are insensitive to thermal fluctuations on cellular length scales. However, we show that intracellular microtubules exhibit bending amplitudes with a surprisingly thermal-like wavevector dependence, but with an apparent persistence length about 100 times smaller than that measured in vitro. By studying the time-dependent bending fluctuations of individual filaments, we find that the thermal-like bends are fluctuating significantly only on short length scales, while they are frozen-in on longer length scales [1], reminiscent of non-ergodic behavior seen in systems far from equilibrium. Long wavelength bends are suppressed by the surrounding elastic cytoskeleton, which confines bending to short length scales on the order of a few microns [2]. These short-wavelength bending fluctuations naturally cause fluctuations in the orientation of the microtubule tip. Tip fluctuations result in a persistent random walk trajectory of microtubule growth, but with a small non-equilibrium persistence length, explaining the origin of quenched thermal-like bends. These results suggest that intracellular motor activity has a highly fluctuating character that dominates over thermal fluctuations, with important consequences for fundamental biological processes.


Tuesday, March 11, 2008 8:00AM - 11:00AM
Session H8 DFD: Focus Session: Glassy Dynamics in Colloids
Morial Convention Center RO6

8:00AM H8.00001 Are colloidal and molecular glass formation related? JOHAN MATTSSON, Chalmers
University of Technology — Understanding why and how a glass is formed on a microscopic level remains an outstanding problem in condensed matter physics. A molecular glass is normally formed by cooling of a liquid. Upon entering the supercooled state, the structural dynamics slows down dramatically and eventually the liquid enters the non-equilibrium glassy state. On route towards the glass, the behaviour shows a range of highly general, near universal characteristics, such as stretched exponential behaviour of dynamic correlation functions and cooperative dynamics. Such generalities exist even though molecular glasses can be formed from liquids encompassing a wide range of molecular structures and interactions. Glass formation also occurs in altogether very different systems. One of the most interesting, both from a fundamental and an applications point of view, is that of colloidal suspensions. There, the binding kinetics of the transient crosslinkers determines the mechanical response of such networks – in the linear as well as the non-linear regime. These effects are important prerequisites for the high adaptability of cells and at the same time might be the molecular mechanism employed by them for mechanosensing.

8:36AM H8.00002 Applications of patchwork dynamics for glassy systems. CREIGHTON THOMAS, ALAN MIDDLETON, Syracuse University, OLIVIA WHITE, MIT — We present work on “patchwork dynamics” as a technique for studying the nonequilibrium properties of glassy systems. In patchwork dynamics, we replace local Monte Carlo simulations, which require exponentially long times to equilibrate at a given length scale, with exact equilibration on patches at a given length scale, which can be done rapidly in models such as the 2D Ising spin glass and disordered dimer models. We have demonstrated some interesting applications of patchwork dynamics to such systems: 1) as a heuristic ground state algorithm for the 2D Ising spin glass on a torus (for which there are no known fast exact algorithms) and the 3D Ising spin glass; 2) as a method to study aging effects, persistence, and memory in 2D and 3D Ising spin glasses; 3) as a sampling procedure to study the nonequilibrium properties of disordered dimer models at finite temperatures.
8:48AM H8.00003 Aging of a Binary Colloidal Glass , JENNIFER M. LYNCH, GIANGUO C. CIANCI, ERIC R. WEEKS, Department of Physics, Emory University — After having undergone a glass transition, a glass is in a non-equilibrium state, and its properties depend on the time elapsed since vitrification. We study this phenomenon, known as aging. In particular, we study a colloidal suspension consisting of micron-sized particles in a liquid — a good model system for studying the glass transition. In this system, the glass transition is approached by increasing the particle concentration, instead of decreasing the temperature. We observe samples composed of particles of two sizes \( d_1 = 1.0 \mu m \) and \( d_2 = 2.0 \mu m \) using fast laser scanning confocal microscopy, which yields real-time, three-dimensional movies deep inside the colloidal glass. We then analyze the trajectories of several thousand particles as the glassy suspension ages. Specifically, we look at how the size, motion and structural organization of the particles relate to the overall aging of the glass. We find that areas richer in small particles are more mobile and therefore contribute more to the structural changes found in aging glasses.

9:00AM H8.00004 Structural signatures of dynamical heterogeneity in supercooled liquids , HEIDI PERRY, DAVID REICHMAN, Columbia University, Department of Chemistry — The underlying mechanism of the transition from liquid to glass is a long-standing open question in condensed matter physics. One long sought after clue to understanding the glass transition is a link between the structure and dynamics of a vitrifying fluid. The dynamics of a supercooled liquid near the glass transition have proven to be collective and heterogeneous, with the length scale of the dynamic regions increasing as the glass transition temperature is approached. Using computer simulations and a normal mode analysis, we demonstrate a link between the structural properties of a super-cooled liquids and the collective dynamical regions.

9:12AM H8.00005 ABSTRACT WITHDRAWN —

9:24AM H8.00006 Fluctuations in the aging regime of a polymer glass\(^1\) , AZITA PARSAEIAN, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University — We perform numerical simulations to investigate the fluctuations in the aging regime of a system of polymers which are interacting via the Lennard-Jones potential. We characterize how the fluctuations evolve by studying (i) probability distributions of local observables such as individual particle displacements \( \Delta x \) and intermediate scattering functions \( C_\ell \) associated with small regions and (ii) dynamic correlation functions such as the four-point density correlation \( g_4(\mathbf{r},t,\mathbf{r},t) \). We find that, similar to small molecule glasses, the probability distributions of local observables approximately collapse when the global two-time correlation \( C_{\text{global}}(t,\mathbf{r},t) \) is held fixed. We test for universality by comparing the probability distributions in the small molecule glass with those in the polymer glass.

\(^1\)Work supported in part by DOE under grant DE-FG02-06ER46300 and by Ohio University.

9:36AM H8.00007 Equipartition theorem in glasses and liquids , VALENTIN A. LEVASHOV, TAKESHI EGAMI , University of Tennessee, RACHEL S. AGA , JAMES R. MORRIS, Oak Ridge National Laboratory — In glasses and liquids phonons have very short life-time, whereas the total potential energy is not linear with temperature, but follows the \( T^{3/5} \) law. Thus it may appear that atomic vibrations in liquids cannot be described by the harmonic oscillator model that follows the equipartition theorem for the kinetic energy and potential energy. We show that the description of the nearest neighbor oscillation in terms of the atomic level stresses indeed provide such a description. The model was tested for various pair-wise potentials, including the Lennard-Jones potential, the Johnson potentials, and only the repulsive part of the Johnson potential. In all cases each of the local elastic energies of the six independent components of the stress tensor is equal to \( kT/4 \), thus the total potential energy is equal to \( (3/2)kT \). Thus this model provides the basis for discussing the thermodynamic properties of glasses and liquids based on atomic excitations. An example of this model leading to the description of the glass transition temperature in metallic glasses is discussed [1].


9:48AM H8.00008 Exceptionally Stable Organic Glasses with Low Enthalpy and High Kinetic Stability Prepared by Vapor Deposition , KENNETH L. KEARNS, STEPHEN F. SWALLEN, M.D. EDIGER, Department of Chemistry, University of Wisconsin-Madison, YE SUN, TIAN YU, LIAN YU, School of Pharmacy, University of Wisconsin-Madison — Vapor deposition can be used to prepare glasses of 1,3,5-(tris)naphthylbenzene (TNB) and indomethacin (IMC) that are much more stable than those created by cooling from the liquid. By vapor deposition we have also been able to create glasses of 1,3,5-(tris)naphthylbenzene (TNB) and indomethacin (IMC) that are much more stable than those created by cooling from the liquid.

10:00AM H8.00009 Magnetic Analogies for the Dynamics of Glass Forming Liquids , JACOB STEVENSON, PETER WOLYNES, University of California San Diego — We present a direct mapping between the dynamics of glass forming liquids and a general random field / random coupling Ising model using the replica effective potential approach. Using the overlap between two structural states of a supercooled liquid we construct a constrained overlap free energy that can be mapped directly onto that of an Ising Hamiltonian. For a Lennard-Jones glass the fluctuations and mean values of the random fields and interactions place it within the universality group of the random field Ising spin glass, not the Ising spin glass. This corresponds with the explanation for a random first order transition.

10:12AM H8.00010 Direct imaging of particle dynamics in attractive colloidal glasses\(^1\) , PIOTR HABDAS, ANDRZEJ LATKA, Department of Physics, Saint Joseph’s University, YILONG HAN, Physics Department, Hong Kong University of Science and Technology, AHMED ALSAYED, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania — We use confocal and fluorescent microscopy to study the dynamics of glassy colloidal suspensions. The suspensions are composed of PMMA colloidal particles in density and index-of-refraction matched liquid and stained with a fluorescent rhodamine dye. A controllable depletion attraction is induced between hard-sphere PMMA particles by adding different amounts of polystyrene polymer to the suspension. Our dynamical measurements focus on jumps experienced by PMMA particles that escape the cage formed by its neighbors. We track these particles over time and correlate particle fluctuations with its changes in average position. We find that as the strength of the attractive potential increases, and the system enters an "attractive liquid" phase, the number of jumping particles increases. We calculate the distribution of particle jump sizes, time between jumps, and spatial distribution of particle jumps; these observations are compared to predictions of molecular dynamics simulations.

\(^1\)This research was supported by an award from Research Corporation.
much more work possibly remains to be done in this important area of space physics. S. Sen et al. Phys. Rev. Lett. 88, 185001 (2002). This article therefore concludes while much work has been done on the ionospheric oscillations much more work possibly remains to be done in this important area of space physics.

10:36AM H8.00012 Accentuated shear thinning of soft sphere suspensions, HANS M. WYSS, Harvard University, JOHAN MATTSSON, Chalmers University of Technology, Sweden, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology, GIOVANNI ROMEO, University of Naples Federico II, Italy, MELAKU MULUNE, Harvard University, ZHIBING HU, University of North Texas, DAVID A. WEITZ, Harvard University — Suspensions of soft colloidal particles exhibit highly unusual rheological behaviors; surprisingly, despite the importance of these materials in a wide range of applications, the underlying physical mechanisms remain poorly understood. Experiments show that suspensions of soft particles exhibit a highly pronounced shear thinning; this decrease in viscosity with increasing shear rate far exceeds the shear thinning observed in suspensions of solid particles. We use soft microgel particles as a model system to elucidate this behavior. Our experimental system allows us to study the mechanical behavior both macroscopically and locally, at the scale of the colloidal particles themselves. We combine data obtained at different length scales to arrive at a simple picture of the observed accentuated shear thinning.

10:48AM H8.00013 Investigation of Rejuvenation and Overaging in Glassy Energy Landscapes, MYA WARREN, JOERG ROTTLER, University of British Columbia — Many glassy systems experience a change in their aging dynamics under the influence of mechanical load. It has long been known that large stresses can cause an apparent decrease in relaxation times (rejuvenation) in polymer glasses, but in colloidal glasses an increase (overaging) has also been observed depending on the strain amplitude. The conditions under which rejuvenation or overaging occur are not yet fully understood. Additionally, there is still considerable controversy over the nature of the resultant states. In order to gain intuition on these outstanding questions, we investigate the aging dynamics under load though stochastic simulations of the Soft Glassy Rheology (SGR) model. For both stress controlled and strain controlled loading, the SGR model exhibits clear regions of overaging and rejuvenation in a parameter space defined by the noise temperature, the quench history, and the strain. Additionally, results show that the states produced under loading are distinct from those that would naturally be visited during aging, and this has effects on the subsequent aging trajectory. Results from the energy landscape picture are compared to pertinent molecular dynamics studies.

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H9 DFD: Instabilities and Fluid Dynamics Morial Convention Center R07

8:00AM H9.00001 Low Frequency Oscillations in the Upper Atmosphere, SUDIP SEN, Kyoto University, Japan & Delhi University, India — No definitive theory exists which explains the origin of various low frequency oscillations observed in the ionosphere. Various authors, over the course of time, have put forward various explanations of this important phenomenon. Most recently it has been proposed that the spatial transverse shear in the parallel flow destabilizes many low frequency oscillations and this may be the origin of low frequency oscillations in the ionosphere [V Gavrishchaka et al., Phys. Rev. Lett. 85, 185001 (2002)]. In this article we review the various theories proposed till date to explain the origin of low frequency oscillations. We address the most recent theories in more detail. We show that the recent proposition of the spatial transverse shear may excite many instabilities may not be so obvious. Parallel flow curvature when taken into account might actually act to stabilize various instabilities [S. Sen et al. Phys. Rev. Lett. 88, 185001 (2002)]. This article therefore concludes while much work has been done on the ionospheric oscillations much more work possibly remains to be done in this important area of space physics.

8:12AM H9.00002 Capillary-controlled instability in immiscible, parallel flow in porous media, THOMAS RAMSTAD, ALEX HANSEN, Department of Physics, NTNU, N-7491 Trondheim and Numerical Rocks AS, Stiklestadaveien 1, N-7041 Trondheim, Norway — When two immiscible fluids flow in parallel in a strongly wetted porous medium the global interface separating them tend to be kept in place by local capillary barriers. However, above a certain threshold in the flow rate, the separating interface may become unstable and mobilized. We study this instability theoretically by using a two-dimensional network as a model for porous media in a flow regime where capillary forces cannot be neglected. It is found that a boundary zone with a sharp saturation profile occurs between the regions originally saturated with either a wetting or a non-wetting phase. This zone has a well defined width and moves with constant speed towards the non-wetting region. In the opposite direction, a current of non-wetting bubbles is set up, but wetting bubbles into the non-wetting region are absent. This behavior is genuinely different from shear-induced Kelvin-Helmholtz instabilities.

1Supported by the Norwegian Research Council

8:24AM H9.00003 Stability of multi-layer Hele-Shaw flows with and without diffusion, PRABIR DARIPA, Texas A&M University — In this talk, we will provide some results in the context of multi-layer Hele-Shaw flows. We will address issues related to collective effects of individually unstable interfaces on the overall stability of multi-layer Hele-Shaw flows in the presence of interfacial surface tensions. We will also discuss complications in the analysis resulting from making, in the above set-up, individual layers also unstable. We obtain some sufficient conditions for suppressing instability of two-layer flows by introducing arbitrary number of constant viscosity fluid layers in between. For stabilization purposes, this condition allows selection of fluids in internal layers based on interfacial surface tensions and viscosities of fluids. Time permitting, we also examine the effects of species diffusion on the stability of the three-layer Hele-Shaw flows. This has relevance to enhanced oil recovery by polymer flooding. Analytically, we will prove the diffusive slow-down of unstable waves. It will be shown that a strong enough diffusion can almost stabilize the flow, though the magnitude of this diffusion coefficient required to completely stabilize the flow will depend on the magnitude of interfacial viscosity jumps and the viscosity gradient of the basic viscous profile of the internal layer. This work has been done in collaboration with Gelu Pasa.
8:36AM H9.00004 Meandering instability of a rivulet on a partially wetting incline. ADRIAN DAERR1, MSC*, Denis-Diderot-University of Paris, LAURENT LIMAT2, MSC*, CNRS & Denis-Diderot-University of Paris — It is common to observe small rivulets in sinks or on window-panes which follow sinuous paths (stationary or not) instead of flowing down along the direction of steepest slope. A laboratory experiment shows that these meandering rivulets exist only for certain ranges of the control parameters (flow rate and substrate inclination). The geometrical properties of the resulting paths can be understood in terms of force balances between inertia, capillarity and contact line pinning. The nature of the instability, i.e. why the straight rivulet becomes unstable, however remains unclear. We study the rivulet near the onset for meandering to understand the role of noise and surface defects.

1CNRS UMR 7057
2CNRS CNRS 7057

8:48AM H9.00005 A quasi 2-D molecular dynamics study of the initiation and evolution of the Kelvin-Helmholtz instability. KYLE CASPERSEN, ROBERT RUDD, DAVID RICHARDS, JIM GLOSILI, Lawrence Livermore National Laboratory, JOHN GUNNELS, IBM, FREDRICK STREITZ, Lawrence Livermore National Laboratory — Typically hydrodynamic phenomena are modeled with continuum mechanics via integration of the Navier-Stokes (NS) equation or a closely related variant. However, as fluids are studied at smaller and smaller length scales atomistic effects can, and will, ultimately dominate; furthermore, even at micron scales it is not clear that the NS equation provides a complete description of the fluid, e.g. due to the initiation of instabilities at the molecular scale in initially quiescent fluids. To assess the effect of atomistic behavior on one particular hydrodynamic phenomenon—the Kelvin-Helmholtz instability—we have performed a very large molecular dynamics simulation of molten metals undergoing shear flow. Nine billion copper and aluminum atoms were sheared at a speed of 2000 m/sec for a total simulated time of more than a nanosecond. We present here results showing the initiation of the instabilities, the crossover to hydrodynamics, and the evolution and scaling behavior of the KH instability in a quasi 2-D geometry. Prepared by LLNL under Contract DE-AC52-07NA27344.

9:00AM H9.00006 A fully 3-D molecular dynamics study of the initiation of the Kelvin-Helmholtz instability. ROBERT E. RUDD, K.J. CASPERSEN, D.F. RICHARDS, J.N. GLOSILI, Lawrence Livermore National Laboratory, J.A. GUNNELS, IBM, F.H. STREITZ, Lawrence Livermore National Laboratory — The modeling of hydrodynamic phenomena has almost exclusively been the purview of continuum mechanics, specifically, through the use of the Navier-Stokes equation and closely related variants. Nevertheless, at the smallest length scales, where atomistic effects become important, it is not clear that this continuum approach provides a complete description of fluid behavior. To understand the effects of atomistics, we have performed a 62.5-billion-atom, fully 3-D molecular dynamics simulation of a cubic micron of molten copper and aluminum. The shear flow at 2 km/s exhibits complex phenomena associated with a Kelvin-Helmholtz (KH) instability. In this presentation we will discuss the initiation and early evolution of the KH instability, focusing specifically on the effects of full atomistic resolution.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

9:12AM H9.00007 Bubble Pinch-off at High Pressures. J.C. BURTON, R. WALDREP, and P. TABOREK, University of California, Irvine — Previously we have studied the pinch-off of conventional air bubbles in water [1]. For inviscid fluids, the shrinking of the neck radius of the bubble can be described by a power-law in time with an exponent close to 1/2. As the density of the interior gas is increased, instabilities are expected to occur in the liquid/gas interface [2]. We present high-speed videos and numerical simulations of the pinch-off of high-pressure gaseous bubbles in and exterior inviscid fluid. The density ratio between the exterior fluid and interior gas is $D=\rho_{ext}/\rho_{int}$. In the simple case of small $D\sim 0.001$, the pinch-off is similar to that of a water drop pinching-off in air, while at large $D\sim 1000$, the pinch-off is that of an air bubble in water. By using sulfur hexafluoride as a working gas, we are able to span a wide ranging of density ratios simply by increasing the pressure of the gas. A high-pressure (~30 atm) chamber with optical access through sapphire windows was constructed in order to view the pinch-off. The numerical simulations are performed assuming perfectly inviscid fluids using boundary-integral techniques. Instabilities in the interface are seen for intermediate density ratios. Comparisons between experimental and numerical results will be discussed.


9:24AM H9.00008 First order phase transition in the height of a meniscus in a tapered capillary. MICHAELA PETTERSEN, Washington and Jefferson College, ETIENNE ROLLEY, Laboratoire de Physique Statistique, Ecole Normale Superieure — When a fluid rises in a capillary of non-uniform cross section, additional terms arise in the balance of capillary forces, compared to the case of a capillary of uniform cross section, due to the changing area of the meniscus. Recently, it has been pointed out that this can lead to a first order phase transition, resulting in a discontinuous jump in the equilibrium position of the meniscus. We present the results of an experiment using isopropanol and silicone oil in cones with apex cross section, due to the changing area of the meniscus.

9:36AM H9.00009 Luminescence from Laser-Induced Bubbles in Water-Glycerol Mixtures: Effect of Viscosity1. ERIN ENGLERT, ALLISON MCCARN, GARY A. WILLIAMS, Dept. of Physics and Astronomy, UCLA — We have studied the luminescence emitted from collapsing laser-induced bubbles in water-glycerol mixtures, as a function of the mixture concentration and applied hydrostatic pressure. The primary effect of increasing the glycerol concentration is to increase the viscosity of the fluid. We find that the pulse duration of the luminescence increases by more than a factor of two as the concentration increases up to 33% by volume, where the viscosity is nearly four time that of pure water. At higher concentrations the pulse duration remains nearly unchanged, until no luminescence can be observed at concentrations above 60% (viscosity greater than 15 times that of water). The pulse duration further increases with applied pressures up to 8 bars, similar to that seen earlier in pure water.

1Work supported by the NSF, DMR 05-48521, and one of us (A. M.) acknowledges support from the UCLA REU program.
H9.00011 A Temporal Period Doubling Route to Spatiotemporal Chaos in a System of Amplitude Equations for the Nematic Electroconvection

10:00AM H9.00011 A Temporal Period Doubling Route to Spatiotemporal Chaos in a System of Amplitude Equations for the Nematic Electroconvection1, JULIANA OPREA, GERHARD DANGELMAYR, Colorado State University — We analyze the transition from periodic solutions to spatiotemporal chaos in a system of four globally coupled Ginzburg Landau equations describing the dynamics of instabilities in the electroconvection of nematic liquid crystals, in the weakly nonlinear regime. If spatial variations are ignored, these equations reduce to the normal form for a Hopf bifurcation with O(2) x O(2) symmetry. Coexistence of low dimensional and extensive spatiotemporal chaotic patterns, as well as a temporal period doubling route to spatiotemporal chaos, corresponding to a period doubling cascade towards a chaotic attractor in the normal form, are also identified and discussed, for values of the parameters including experimentally measured values of the nematic I52.

1Research supported by NSF/DMS-407418.

H9.00012 Angular momentum transport in complex fluids1, XIAOYU ZHENG, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, MICHAEL SHELLEY, Courant Institute of Mathematical Sciences, NYU — When dyes are dissolved in nematic liquid crystals, the light intensity required for the optical Freedericksz transition can be dramatically decreased. This is due to the torque exerted by the dye on the liquid crystal. The dye molecules absorb light energy and rotate; torque balance is mediated by angular momentum transport from the cell walls via shear flow generated by the rotation [1]. We present a model which accounts for the transport of angular momentum caused by singular vortices present in these complex fluids. The singular vortices generate flow, and are transported by the flow which they generate. For simple fluids, the distribution of vorticity satisfies the biharmonic equation in the Stokes limit, which can be solved analytically. In the case of the non-Newtonian fluids, such as liquid crystals, Leslie-Ericksen continuum theory is used to describe the interactions between the rod-like molecules. [1] P. Palffy-Muhoray, T. Kosa and Weinan E, “Brownian Motors in the Photoalignment of Liquid Crystals”, Appl. Phys. A 75, 293-300 (2002).

1This work was supported by the NSF under grant DMR 0606357.

H9.00013 Particle Dynamics in Bi-Disperse Liquid Fluidized Beds, PHIL SEGRE, Emory University Physics Dep, GARY L. HUNTER, JAMES DAVIDHEISER, ELIZABETH BAKER, Emory Univ. Physics Dep. — We study particle velocities and concentration profiles of mixtures of 2 different sized particles in concentrated liquid fluidized beds. For binary systems of particles of the same density, we find that there is always a complete phase separation in the bed. The larger particles occupy a zone in the lower part of the bed, and the smaller ones a zone in the upper part. For binary systems of particles of different density materials, conditions are found where the binary particles are either fully separated, partially mixed together, and at a single point called the inversion point, fully mixed into a one phase state. Results will be presented on the phase diagrams of several binary suspensions as well as the properties of the velocity fluctuation magnitudes and spatial correlation lengths.

H9.00014 Polygonal hydraulic jump on microtextured surfaces, EMILIE DRESSAIRE, LAURENT COURBIN, SEAS, Harvard University, JEROME CREST, Dept. of Mechanical Engineering, MIT, HOWARD A. STONE, SEAS, Harvard University — Fluid motion can be drastically influenced by the nature of boundaries. For instance, we have shown recently [1] that a substrate with a regular array of micron-size posts can cause partially wetting fluids to take on polygonal shapes. Here, we report on the hydraulic jump that occurs when a water jet impinges a topographically patterned surface, i.e. an array of micron-size posts arranged on square or hexagonal lattice. By varying the topographic features (shape and height of the posts, lattice distance) and the jet properties (size of the nozzle, flow rate), we obtain a variety of stable shapes including hexagons, eight corner stars and circles. We rationalize our results by taking into account a fluid velocity that depends on the orientation of the lattices.


H9.00015 Enstrophy-constrained stability analysis of beta-plane Kolmogorov flow with drag, YUE-KIN TSANG, WILLIAM YOUNG, Scripps Institution of Oceanography, UCSD — For forced two-dimensional flows, energy injected at a certain wavenumber is redistributed to both larger and smaller wavenumbers. This results in a constraint on the time evolution of the difference between the energy and enstrophy. By incorporating this constraint in an energy stability analysis of Kolmogorov flow on a beta-plane with drag, we establish an extended region in the parameter space of beta and the drag coefficient where the flow is stable to arbitrary perturbations. Complementary to this nonlinear stability result, linear instability theory is used to determine the part of the parameter space where the flow is unstable to infinitesimal perturbations. We also find that the most unstable mode in the linear stability analysis has a discontinuous change in structure as beta decreases below a certain value. Results from numerical simulations spanning the parameter space support the theoretical predictions.

Tuesday, March 11, 2008 8:00AM - 11:00AM
Session H10 DCMP: Josephson Effects Morial Convention Center RO8
8:00AM H10.00001 Suppression of macroscopic quantum tunneling in a large Josephson junction coupled to a resonator\(^1\), BRAD TREES, Ohio Wesleyan University, JOSHUA SCHIFFRIN, Carnegie-Mellon University, YASER HELAL, Ohio Wesleyan University, BRIAN SILLER, University of Illinois at Urbana-Champaign — We calculated the zero-temperature macroscopic quantum tunneling rate of a current-biased Josephson junction weakly coupled to a resonator. We allow for the effects of environmental dissipation on both the junction and the resonator, and we consider both cases of weak and strong junction damping. We find that coupling to the resonator has a suppressive effect on the junction’s tunneling: the stronger the coupling strength between the junction and resonator, the greater the reduction of the tunneling rate. Including damping to the junction also suppresses tunneling, but damping the resonator partially counteracts the suppression provided directly by the junction-resonator coupling. Modeling the dependence of the junction-resonator coupling on the resonator’s frequency \( \omega_R \) in a power law fashion \( U_{int} \propto (\omega_R)^{n} \), we find that for \( 0 < n < 1 \) the tunneling rate exhibits a nonmonotonic dependence on \( \omega_R \), and for \( n = 1/2 \), the tunneling rate is maximally suppressed for \( \omega_R/\omega_1 \approx 1 \), where \( \omega_1 \) is the bias current-dependent plasma frequency of the junction.

\(^1\)Work supported by the National Science Foundation (REU/RET grant #0648751) and Ohio Wesleyan University.

8:12AM H10.00002 Identifying the Odd-Frequency Superconducting State by a Field-Induced Josephson Effect\(^1\), JACOB LINDER, Norw Univ of Sci & Tech, TAKEHITO YOKOYAMA, University of Nagoya, ASLE SUDBO, Norw Univ of Sci & Tech — The prevalent symmetry in known superconductors may be described as odd under exchange of spin coordinates, and even under an exchange of spatial or time coordinates of the electrons constituting the Cooper pair. However, other types of pairing are also permitted by the governing Pauli principle. Among these is the so-called odd-frequency pairing state, which has been predicted to arise both in N/S and F/S proximity systems. Extending the possible pairing states compatible with the Pauli-principle will likely have impact on a wide range of sub-disciplines in physics, ranging from astrophysics to extremely compressed quantum liquids. Recent experiments report that such an odd-frequency superconducting bulk state may be realized in certain heavy-fermion compounds. While the Josephson current normally only flows between superconductors with the same symmetry with respect to frequency, we demonstrate that an exchange field may induce a current between diffusive even- and odd-frequency superconductors. This suggests a way to identify the possible existence of bulk odd-frequency superconductors.

\(^1\)Work supported by the Research Council of Norway.

8:24AM H10.00003 Tunable current-phase relation in double-dot Josephson junctions, JENS KOCH, KARYN LE HUR, Departments of Physics and Applied Physics, Yale University — The current-phase relation \( I(\phi) \) of a Josephson junction contains information about the microscopic nature of the Cooper pair transfer. In particular, junctions more complicated than the single tunnel junction exhibit characteristic non-sinusoidal forms. Here, we investigate the Josephson effect in a superconducting double dot device, similar to the devices studied experimentally by Y. A. Pashkin et al. [1] and E. Bibow et al. [2]. In the vicinity of a charge degeneracy line, the system reduces to a two-level system equivalent to a charge qubit. In this regime, we find that the interplay between sequential tunneling and cotunneling of Cooper pairs leads to a strongly non-sinusoidal current-phase relation, tunable via gate electrodes. We propose the measurement of \( I(\phi) \) in a SQUID configuration, analyze the implications of flux noise, and compare our results to different types of Josephson junctions such as single-dot systems and microbridges. [1] Y. A. Pashkin et al., Nature (London) 421 (2003), 823 [2] E. Bibow, P. Lafarge, L. Lévy, Phys. Rev. Lett. 88 (2002), 017003

8:36AM H10.00004 Spontaneous spin accumulation in singlet-triplet Josephson junctions, KRISHNENDU SENGUPTA, TCMP division, Saha Institute of Nuclear Physics, Kolkata, India, VICTOR YAKOVEDNO, Department of Physics, University of Maryland — We show that the Andreev bound states in Josephson junctions between singlet \( s \)-wave and triplet \( p \)-wave superconductors carry a net magnetic moment. This magnetic moment depends on the relative phase between the superconductors constituting the junction and changes sign when the relative phase shifts by \( \pi \). We estimate the net magnetization of such junctions and suggest several realistic experiments to detect this magnetization. We also discuss possible magnetization flip in such junctions in the presence of an applied bias voltage.

8:48AM H10.00005 Small Josephson junctions in asymmetric SQUIDs, DAN SULLIVAN, Department of Physics, University of Maryland, College Park, TAUNO PALOMAKI, MARK GUBRUD, MICHAEL DREYER, BARRY BARKER, JAMES ANDERSON, CHRIS LOBB, FRED WELLSTOOD — Ultra-small Josephson junctions are known to be susceptible to quantum fluctuations in the phase difference across the junction, resulting in an effective suppression of the critical current. We have investigated a method for stabilizing this phase difference by shunting a small junction (with a critical current \( I_{01} \approx 1 \text{nA} \)) with an additional capacitance and incorporating the junction in a dc SQUID loop. The second junction in the \( \text{Al/AlO}_x/\text{Al} \) SQUID has a much larger critical current \( I_{02} \approx 1 \text{µA} \), producing a SQUID that is highly asymmetric. Our results show that the SQUID inductively couples the phase differences of the large and small junctions, leading to reduced phase fluctuations, and thus allowing accurate measurement of the small junction’s critical current at millikelvin temperatures. This work was supported by the National Science Foundation and the Laboratory for Physical Sciences.

9:00AM H10.00006 Scanning Josephson Tunneling Microscopy of Single Crystal Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{8+\delta}\) from a Conventional Superconducting Tip, HIKARI KIMURA, University of California, Berkeley, RICHARD BARBER, Santa Clara University, SHIMPEI ONO, CRIEPI, YOICHI ANDO, Osaka University, ROBERT DYNES, University of California, Berkeley and LBNL — Using a scanning tunneling microscope with superconducting Pb-coated tips (S-STM), we have observed the thermally fluctuated Josephson Effect between the tip and conventional superconductors. Such STM-based Josephson junctions are a powerful tool that can directly probe the phase of the superconducting condensate via the Josephson Effect as well as characterize the quasiparticle spectrum, both on a nanometer length scale. In this talk we present data from Josephson junctions formed between the S-STM tips and Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{8+\delta}\) Single crystals. These results clearly show \( s \)-axis Josephson tunneling between a conventional superconductor and both overdoped and optimally doped Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{8+\delta}\). Josephson measurements at various surface locations indicate an inhomogeneous structure of the \( I_{c}R_N \) product in overdoped Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{8+\delta}\). These local \( I_{c}R_N \) data of the Bi\(_2\)Sr\(_2\)Ca\(_2\)Cu\(_3\)O\(_{8+\delta}\) are related to the local superconducting gap. This work is supported by DOE Grant No. DE-FG02-05ER46194.

9:12AM H10.00007 Thermal Management in Large Bi2212 Mesas used for Terahertz Sources\(^3\), C. KURTER, K. E. GRAY, Q. LI, Argonne National Laboratory, L. OZYUZER, Izmir Institute of Technology, A. E. KOSELEV, Argonne National Laboratory, T. YAMAMOTO, K. KADOWAKI, University of Tsukuba, U. WELP, Argonne National Laboratory — We report the intrinsic tunneling characteristics of 300x100x1\( \mu \)m\(^3\) mesa on Bi2212 single crystals that have recently shown high-power emission at terahertz frequencies due to the ac Josephson effect. Despite the large mesa volumes compared to those of others, there is an accessible range of voltages for which self-heating does not exceed \( T \). A temperature increase proportional to power, \( P=IV \). We find that the local temperatures along the nonlinear I(V) are consistent with the observed unpolarized thermal radiation from the mesa, thus verifying the model.

\(^3\)Supported by U.S. DOE Basic Energy Science, Contract No. DE-AC02-06CH11357
9:24AM H10.00008 Quantized energy levels in quantum and classical regimes in current-biased intrinsic Josephson junctions, MYUNG-HO BAE, MITRABHANU SAHU, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3080, USA, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea, ALEXEY BEZRYADIN, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3080, USA, HU-JONG LEE COLLABORATION — The multiphoton transitions between quantized energy levels in the current-biased $\text{Bi}_x \text{Sr}_y \text{Sr}_z \text{Ca}_u \text{Cu}_v \text{O}_{w+z}$ intrinsic Josephson junctions (IJJs) in the quantum and classical regimes are studied through the switching current distributions. The system shows the saturation behavior of the switching current distributions near $T_c \sim 0.8$ K, which is the crossover temperature between classical and quantum nature of the system. We observe the multiphoton transitions between quantized energy levels in the quantum regime, which is manifested by the enhancement of the escape rate in the microwave radiation with frequencies of 12-16 GHz. This enhancement behavior keeps even in the classical regime and is washed out near $T_c \sim 2$ K, of which thermal energy corresponds to the energy level spacing at the switching currents. This means that the existence of the quantized energy levels even in the classical regime of IJJs, due to the relatively large plasma frequency in the IJJs.

9:36AM H10.00009 Direct observation of a $\sin(2\phi)$ component in the current-phase relation of superconductor-ferromagnet-superconductor (SFS) Josephson junctions, M.J.A. STOUTIMORE, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL USA, A.YU. RUSANOV, Laboratory of Superconductivity, ISSP-RAS, Chernogolovka, Russia, D.J. BAHR, V.A. OBOZNOV, V.V. BOLGINOV, A.N. ROSSOLENKO, V.V. RYAZANOV, D.J. VAN HARLINGEN — We present direct measurements of the current-phase relation (CPR) of SFS Josephson junctions in an rf-SQUID geometry. The junctions are fabricated from $\text{Nb-Cu}_{17} \text{Ni}_{13}-\text{Nb}$ trilayers with a junction area of $2 \times 2 \mu \text{m}^2$ and a CuNi thickness of 7 nm. By measuring the magnetic flux through the rf-SQUID as a function of applied current, we observe transitions between an arbitrary $\phi$-Josephson junction state and a $\phi$-junction state characterized by a phase difference of $\pi$ in the ground state occurring at temperatures between 1.5 K and 3.5 K. Near this temperature crossover, we observe period-doubling of the CPR indicating the existence of a term proportional to $\sin(2\phi)$. Work is underway to determine if this signifies an intrinsic second-order tunneling mechanism or is the result of junction inhomogeneities.

9:48AM H10.00010 Sub-Gap Currents in Nb/Al/AOx/Nb Josephson Junctions and Their Dependence on the Method of Barrier Formation, PAUL B. WELANDER, TIM J. MCARDLE, STEPHANIE LAW, JAMES N. ECKSTEIN, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 — Josephson tunnel-junctions have been fabricated using two different methods of barrier formation. Both types of devices start with single-crystal Nb/Al bi-layers grown by molecular beam epitaxy on A-plane sapphire. It is found that complete wetting of the Nb layer is achieved with 20 nm of Al evaporated at room temperature. The barrier is then formed either by thermal oxidation of the Al surface in molecular oxygen (the well-known process developed by Gurvitch et al.) or by co-deposition Al in an oxygen background of about 5 micro-torr. A Nb counter-electrode is deposited in situ by evaporation at room temperature. Josephson junctions fabricated from these multi-layers exhibit Fiske resonances and a reduced gap voltage due to the relatively thick Al layer. For devices tested at 4 K, the co-deposition process yields junctions that show a sub-gap current in agreement with theory and no measurable shunt conductance. In contrast, those devices with barriers formed by thermal oxidation show a small shunt conductance in addition to the predicted sub-gap current.

1Presently at MIT Lincoln Laboratory, Lexington, MA 02420

10:00AM H10.00011 Ferromagnetic Josephson Junctions, TRUPTI KHAIRE, WILLIAM PRATT, NORMAN BIRGE, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824 — Superconducting correlations cannot penetrate into a ferromagnet over a large distance due to the pair breaking effect of the exchange field. Ferromagnet/Superconductor (F/S) systems are often studied using weak ferromagnetic alloys with smaller exchange energy and correspondingly larger penetration depth. We are studying F/S junctions with the weak ferromagnetic alloy, CuNi [1]. The samples are fabricated by sputtering the S/F/S trilayer onto a Si substrate; they are subsequently patterned using trilayer photolithography and ion milling to obtain pillars of 50 micron diameter. Measurements performed on these pillars at 4K show the Josephson effect with the expected modulation of the critical current as a function of applied magnetic field. Because spin-flip scattering and spin-orbit scattering are strong in weak ferromagnetic alloys such as CuNi, there is an incentive to work with strong ferromagnets. The results from our CuNi data confirm the robustness of the sample fabrication technique and pave the way to future studies of Josephson junctions with strong ferromagnets such as Ni. [1] V. A. Oboznov, Phys. Rev. Lett. 96, 197003 (2006)

1This work is supported by US-DOE grant, DE-FG02-06ER46341.

10:12AM H10.00012 I-V Characteristics vs. Spatial Dissipation Maps in YBCO Grain Boundary on Bicrystal Substrates, CHUHEE KWON, MEGUMI YAMAMOTO, SAMUEL POTTISH, California State University Long Beach, TIMOTHY HAUGAN, PAUL BARNES, Air Force Research Laboratory, CALIFORNIA STATE UNIVERSITY LONG BEACH COLLABORATION, AIR FORCE RESEARCH LABORATORY COLLABORATION — Grain boundary (GB) properties of YBCO films on SrTiO3 bicrystal substrates with 24 degree misorientations are examined by transport and scanning laser microscopy (SLM) techniques. Thermoelastic SLM clearly shows the location of grain boundaries, and variable temperature SLM confirms that GB has lower Tc. A series of I-V measured in superconducting states exhibit clear step-like features identified in earlier papers as sub-gap structures. The low temperature SLM shows a close relation between the step-like features and the local dissipation pattern in GB. We believe that the activation of Fiske steps is responsible for the step-like I-V, and SLM images show the spatial pattern of the self-excited resonance in GB. We will also discuss how Ca-doping and nanoparticle additions on YBCO affect the junction properties.

1The work was supported by AFOSR.

10:24AM H10.00013 Vibronic Effects in Superconducting Niobium Nanowires, BRANDON DONEHOO, ZHENTING DAI, ALEXEI MARCENKOV, Georgia Institute of Technology — Research of superconducting transport through microscopic objects with intrinsic vibrational degrees of freedom is a frontier research avenue. Here we report on experimental studies of a few-atom niobium nanowires prepared in a mechanically-controlled break junction set-up. We present evidence for the resonant interaction between the ac Josephson effect and the mechanical motion of atoms in niobium dimer nanowires at frequencies up to about 8 THz. This is application-rich, but a largely unexplored frequency range ("teraertz gap"), which interrogates the lowest frequency vibrational modes of complex organic and biological molecules. We also discuss superconducting transport and noise in niobium nanowires with oxygen contamination.

1Work performed in collaboration with C. Zhang, R. Barnett, and U. Landman (Georgia Institute of Technology). Work supported by the NSF CAREER Grant No. DMR-0349110.
10:36AM H10.00014 Fluxon dynamics in a Josephson junction parallel array\textsuperscript{1}, NIKHIL FERNANDES, KENNETH SEGALL, USHNISSH RAY, Colgate University, ADAM DIOGUARDI, University of California at Davis — We present experimental measurements on the dynamics of fluxons in an array of Josephson junctions. Fluxons trapped in a parallel array of Josephson junctions upon cooldown experience a potential determined by the junction critical currents and the cell inductances. We probe the dynamics of the fluxon with switching current measurements, which allow determination of the transition rate of the fluxon from its pinned state to a running state. The transition to the running state is initiated by thermal activation at temperatures higher than the quantum crossover temperature for the junctions. Below the crossover, we observe an abrupt change in the critical force needed to move the fluxon. Quantum tunneling of the fluxons is a possible explanation for this observation. We present the data, numerical simulations, and a discussion of the results.

\textsuperscript{1}Funding from NSF Grant DMR 0509450

10:48AM H10.00015 Field-dependence of interlayer tunnelling in Bi$_2$Sr$_2$CaCu$_2$O$_8$, TIMOTHY BENSEN-MAN, JOHN COOPER, University of Cambridge, GEETHA BALAKRISHNAN, University of Warwick — Micron-scale ‘mesa’ structures fabricated on the surface of single crystals of strongly anisotropic high-temperature superconducting (HTS) compounds form stacks of ‘intrinsic Josephson junctions’ connected in series. Studying the current-voltage ($I$-$V$) characteristics of HTS mesa is now an established technique for obtaining important information regarding the electronic density of states ($\rho_D$) in these compounds, such as the magnitude $\Delta$ of the superconducting energy gap, and its symmetry in $k$-space. We have fabricated mesas on the HTS compound Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi-2212) and studied these at a range of hole-doping levels, temperatures, and applied magnetic fields. Of particular interest is the field-dependent behaviour of the $I$-$V$ characteristic at bias voltages much less than the sum-gap voltage $2\Delta/e$, corresponding to quasiparticles near the gap nodes. We compare our results with predictions for the field-dependent DoS made by Volovik \cite{1} in which the local energy is assumed to be Doppler shifted by the local superfluid velocity. We also discuss features seen in our tunnelling characteristics at voltages above $2\Delta/e$, which may correspond to strong-coupling effects in Bi-2212.\cite{1, 2, 3}


\cite{3} S. Curtarolo \textit{et al}, JETP Letters 80, 272 (2004).

\textbf{Tuesday, March 11, 2008 8:00AM - 11:00AM –}

\textbf{Session H11 DMP: Focus Session: MgB2-like: Computational Design of Novel Superconductors}

\textbf{Morial Convention Center R09}

8:00AM H11.00001 Quasi-two-dimensional electronic states in a dense three-dimensional Li-Be alloy\textsuperscript{1}, RICHARD G. HENNIG, Cornell University, JI FENG, Harvard University, ROALD HOFFMANN, N.W. ASHCROFT, Cornell University — High pressure can affect electronic structure and crystal packing, and in some cases even induce compound formation between elements that do not bond under ambient conditions. Our computational study for the Li-Be system shows that the reactivity of Li and Be is fundamentally altered by pressure. These two lightest metallic elements are immiscible at ambient conditions. Using structure search methods we discover four stoichiometric Li-Be compounds that are stable over a range of pressures. The electronic density of states of one of them displays a remarkable step-like feature and plateau at the bottom of the valence band, which is typical of a quasi-2D electronic structure and rather unexpected in a 3D crystal environment. We attribute this feature to large size differences between the ionic cores of Li and Be. Under increased pressure, the Li cores start to overlap and thereby expel valence electrons into quasi-two-dimensional layers characterized by delocalized free-particle-like states in the vicinity of Be ions. These alloys are also interesting from the perspective of superconductivity. The $T_c$ in the LiBe alloy is expected to be substantially higher than the component elements due to the increased density of states at the Fermi energy compared particularly to elemental Be.

\textsuperscript{1}Supported by the National Science Foundation and the Petroleum Research Fund of the American Chemical Society

8:12AM H11.00002 First-principles search for potential high temperature superconductors in the Mg-B-A (A=alkaline metal) system with high boron content\textsuperscript{1}, ROMAN CHEPULSKYY, Duke University, IGOR MAZIN, Naval Research Laboratory, STEFANO CURTAROLO, Duke University — Possible superconductivity at 50K was recently reported \cite{1} in the Mg-B-A (A=Ca, Sr, Ba) system. Although attempts to reproduce this finding have been unsuccessful so far \cite{2}, if a stable or metastable phase could be found by a first principle search similar to that in Ref. 3, this would have lent credence to the experimental finding \cite{1} and outline possible further directions. The results of Ref. 1 suggest that (a) the superconducting phase is not similar to MgB$_2$ (B site has cubic or similarly high symmetry) and (b) boron content is higher than in MgB$_2$. We report first-principles study of the thermodynamics of alkali and alkaline earth doping in the boron-rich part of the Mg-B phase diagram (MgB$_n$, with $n>2$) searching for a phase that could explain the results of Ref. \cite{1}.\cite{1} A. V. Palenichenko \textit{et al}, JETP Letters 86, 064510 (2007). \cite{2} R K Singh \textit{et al} http://arxiv.org/abs/0709.4001v1. \cite{3} S. Curtarolo \textit{et al}, \textit{Calphad} 29, 163 (2005).

\textsuperscript{1}Research was supported by ONR and NSF

8:24AM H11.00003 Engineering superconductors with ab initio methods: ternary metal borides, ALEKSYE KOLMOGOROV, University of Oxford, MATTEO CALANDRA, STEFANO CURTAROLO — We have performed a targeted search for novel superconducting ternary borides starting from the recently identified class of binary metal sandwich (MS) structures \cite{1}. Our \textit{ab initio} calculations suggest that a theoretically-devised MS lithium monoboride gains in stability when alloyed with electron-rich metals \cite{2,3}. In an effort to pre-select compounds with the strongest electron-phonon coupling we evaluate the softening of the in-plane boron phonon mode in a large class of metal borides. Our results reveal interesting general trends for the in-plane boron phonon modes as a function of the boron-boron bond length and the valence of the metal \cite{4}.\textit{Research supported by ONR and NSF.} \cite{1} PRB 73, 180501(R) (2006) \cite{2} PRB 74, 224507 (2006). \cite{3} PRB 75, 144506 (2004) \cite{4} A.N. Kolmogorov, M. Calandra, S. Curtarolo, submitted to PRB.

8:36AM H11.00004 Electron-Phonon interaction in hexagonal layered compounds, LILIA BOERI, MPI-KFK, Stuttgart, MATTEO GIANTOMASSI, UPCM, Universit`a `La Sapienza`, Roma, Italy, OLE KROGH ANDERSEN, MPI-KFK, Stuttgart, Germany — The discovery of superconductivity in MgB$_2$ has initiated a thorough search for new electron-phonon ($e-\phi$) superconductors, particulary among hexagonal layered compounds. In this talk I will describe, using \textit{ab initio} methods, the factors that determine the electron-phonon properties of two classes of recently discovered superconductors, namely alkali-earth intercalated graphites (highest $T_c$, 15.1 K for CaC$_2$)\cite{1} and metal-intercalated ternary compounds MaAlSi.\cite{2}


8:48AM H11.00005 Structure and Superconductivity of Calcium under Pressure, Z. P. YIN, Dept. of Physics, UC Davis, F. GYG, Dept. of Applied Science, UC Davis, W. E. PICKETT, Dept. of Physics, UC Davis — The structure, phonon spectrum and electron phonon coupling of Ca under pressure is studied by first principle calculations. Experimentally, Ca at room temperature is simple cubic (SC) at pressure between 30 GPA and 109 GPA and goes to unknown structure above 109 GPA. Its superconducting $T_c$ increases significantly in the SC phase, increasing to 23 K at 109 GPA (25 K at 161 GPA). Linear response calculations reveal that SC Ca is horribly unstable in the corresponding pressure range (at $T=0$). Ab initio molecule dynamics calculations on a $4\times4\times4$ supercell find the SC phase is distorted into a four-atom bcc structure that is dynamically stable in the 40-110 GPA range. At even higher pressure, this bcc structure becomes dynamically unstable (imaginary frequencies). T. Ishikawa et al. (private communication) proposed an orthorhombic structure around 120 GPA. We confirmed this structure with minor differences of internal parameters. The theoretical x-ray diffraction (XRD) pattern of this structure has very good match with the experimental XRD pattern of the Ca V phase. Our linear response calculations further confirm that it is dynamically stable, and indications of strong electron-phonon coupling in this phase will be presented.

9:00AM H11.00006 Constraints on $T_c$ for superconductivity in heavily boron-doped diamond, JONATHAN E. MOUSSA, MARVIN L. COHEN, UC Berkeley & LBNL — Calculations of electron-phonon coupling are performed for boron-doped diamond structures without electronically compensating defects over a wide range of boron concentration. The effects of boron substitutional disorder are incorporated through the use of randomly generated supercells, leading to a disorder-broadened distribution of results. After averaging over disorder, this study predicts a maximum bulk $T_c$ near 55 K for boron concentrations between 20% – 30%, assuming the validity of the simple structural model used and a Coulomb pseudopotential of $\mu^* = 0.12$. Considering only the largest electron-phonon coupling values of the distribution, superconductivity may still percolate through the material at higher temperatures, up to 80 K, through the regions of large coupling. A synthesis path is proposed to experimentally access this class of materials.

9:12AM H11.00007 Superconductivity in high-pressure solids, JOHN S. TZE, Department of Physics and Engineering, University of Saskatchewan, Saskatoon, SK S7N 5E2, Canada — The structural principle behind the unusual features in the high-pressure phases of simple alkali elements is reviewed. It is shown that there exists a pressure regime in which the elemental solids are likely to adopt a layer structure. There are two novel characteristics associated with this structure type. The system tends to be at the proximity of phonon and electronic instabilities. The combined effect is a significant enhancement of electron-phonon coupling, resulting in a superconducting state. We demonstrate this empirical observation with selected examples including a recently predicted novel high pressure structure of SH$_4$ which shows very high superconducting critical temperature.

9:48AM H11.00008 Layered Structures Favor Superconductivity in Compressed Solid SiH$_4$, HAI-QING LIN, Chinese University of Hong Kong, XIAO-JIA CHEN, Carnegie Institute of Washington, JIANG-LONG WANG, Chinese University of Hong Kong, VIKTOR V. STRUZHKIN, HO-KWANG MAO, Carnegie Institute of Washington — The electronic and lattice-dynamics properties of compressed solid SiH$_4$ have been calculated over the pressure regime up to 300 GPA with density functional theory. We find that the structures having layered network with eight-fold SiH$_4$ coordination favor the metallization and superconductivity. The layered $\text{Cs}$SiH$_4$ is predicted to have a superconducting transition temperature of 75 K at 70 GPA and opening new possibilities for exploring high temperature superconductivity in the hydrogen-rich system.

10:00AM H11.00009 First-Principles Study of Superconductivity in boron-doped SiC, JESSE NOFFSINGER, FELICIANO GIUSTINO, STEVEN LOUIE, MARVIN COHEN, UC Berkeley — The discovery of superconductivity in materials such as intercalated graphite, alkali-doped fullerences, and boron-doped diamond has drawn significant interest to carbon-based superconductors. Recent experiments indicate that boron-doped cubic SiC may superconduct above 1 K. [1]. We investigate the superconductivity in cubic SiC using a first-principles approach. We describe the electronic structure within density functional theory and the lattice dynamics within density functional perturbation theory. The electron-phonon interaction matrix elements are calculated via a recently developed method based on Wannier functions [2]. The boron doping is accounted for by a virtual crystal approximation. In addition to the coupling of Fermi surface electronic states to optical phonon modes, there appears to be a non-negligible contribution to the electron-phonon coupling arising from acoustics phonons. Superconductivity is discussed by analyzing the similarities and the differences with respect to the closely related boron-doped diamond. [1] Z-A. Ren et al. private communication. [2] F. Giustino et al. Phys. Rev. B 76, 165108 (2007)

10:12AM H11.00010 First principles study of Al and C-doped MgB$_2$: evolution of two gaps and critical temperature, OMAR DE LA PEÑA-SEAMAN, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, ROLF HEID, KLAUS-PETER BOHNEIN, Institut fuer Festkoerperforsch. Forschungszentrum Karlsruhe, Germany — We have studied the electronic-phonon and superconducting properties of the Mg$_{1-x}$Al$_x$B$_2$ and Mg$_{1-x}$B$_2$(1-x)C$_{2x}$ alloys within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloys. For both systems, the Eliashberg spectral function $(\alpha^2 F(\omega))$ and the electron-phonon coupling parameter $(\lambda)$ have been calculated in the two band model $(\sigma,\pi)$ for several concentrations until $(\lambda/AI) = 0.55$ and $(x(C) = 0.175)$. Using the calculated $\lambda^2 F(\omega)$ and a diagonal expression for the Coulomb pseudopotential matrix, $\mu^*$, we solved numerically the Eliashberg gap equations in the two band model without interband scattering. We reproduce the experimental decreasing behavior of $\Delta_{\sigma}(x)$, $\Delta_{\pi}(x)$, and $T_c(x)$ for both alloy systems. The role of the interband scattering in the observed behavior of the superconducting gaps and $T_c$ in the Al- and C-MgB$_2$ alloys is discussed. This research was supported by Consejo Nacional de Ciencia y Tecnologia (Conacyt) under Grant No. 45360-F.

10:24AM H11.00011 Effects of Quenched Random Gap Inhomogeneities on the Specific Heat of a Model High-$T_c$ Superconductor, DAVID STROUD, Department of Physics, Ohio State University, Columbus, OH 43210, DANIEL VALDEZ-BALDARES, Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — In many cuprate superconductors, scanning tunneling microscopy experiments show that the energy gap has substantial quenched random spatial variations. We have calculated how such gap variations affect the specific heat $C_V$ in a model for the most anisotropic of these materials. The model is based on a Ginzburg-Landau free energy functional in which position-dependent coefficients are used to model quenched inhomogeneity. Using Monte Carlo simulations, we evaluate $C_V$ for different disorder strengths. Near optimal doping, we find that quenched gap disorder substantially broadens the specific heat anomaly near the phase ordering transition $T_s$, compared to that due to thermal fluctuations alone. But for strongly underdoped samples, in which $T_c$ is greatly separated from the pseudogap temperature $T_p$, disorder only slightly increases the broadening beyond the already substantial amount due to thermal fluctuations. We compare these results to recent experiments.

1Supported by NSF and DOE.
The temperature dependent gap edge in strong-coupling superconductors

10:48AM H11.00013 A DFT study of the UCoGe magnetic superconductor, PABLO DE LA MORA, Fac. de Ciencias, UNAM, Mexico, ORACIO NAVARRO, Inst. Inv. Materiales, UNAM, Mexico — Recently Huy et al. (PRL 99, 067006) found that UCoGe is a superconductor coexisting with magnetism. Electronic structure calculations were performed on this compound using the WIEN2k package, results show that its magnetism is anisotropic, with the easy magnetic axis in the c-direction. The magnetic moment of the U atom is quite small, but there is a large moment in the Co atom which is in disagreement the experimental result of Huy et al. These results contrast with the isostructural magnetic superconductor URhGe, in which compound the U-atom moment is relatively large; while for the Rh atom it is small. The main contribution at E_F is due to U-5f and Co-3d. Ge has little contribution. There are many similarities with the MgB2 superconductor, there are many bands at E_F and UCoGe has a distorted MgB2 crystalline structure, but the superconductivity mechanism seems to be of different origin.

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H12 DCMP: Lattice and Magnetic Properties of Multiferroics Morial Convention Center 203

8:00AM H12.00001 Infrared phonon dynamics of multiferroic BiFeO3 single crystal, R.P.S.M. LOBO, CNRS-ESPCI, Paris, France, R.L. MOREIRA, Depto. Fisica, UFMG, Belo Horizonte, MG, Brazil, D. LEBEUGLE, D. COLSON, DSM/DRCAM/SPEC, CEA, Saclay, France — We discuss the first infrared reflectivity measurement on a BiFeO3 single crystal between 5 K and room temperature. The predicted ab-plane E phonon modes are fully and unambiguously determined. The frequencies of the 4 A1 c-axis phonons are found. These results settle issues between theory and data on ceramics. Our findings show that the softening of the lowest frequency E mode is responsible for the temperature dependence of the dielectric constant, indicating that the ferroelectric transition in BiFeO3 is soft-mode driven.

8:12AM H12.00002 Electromagnons and Multiple Phase Transitions in BiFeO3 Multiferroic System, MARIOLA RAMIREZ, A. KUMAR, S. DENEV, J. IHELEFED, D. SCHLOM, VENKATRAMAN GOPALAN, Penn State University, R. RAI, X. XIU, J. MUSEFELDT, University of Michigan, S. LEE, S. CHEONG, Rutgers University, R. RAMESH, J. SEIDEI, E. CHIU, J. ORESTEIN, University of California, Berkeley — Magnetoelastics (ME) multiferroics has recently become an exciting research area due to its potential technological applications. Of special relevance is the case of Bismuth ferrite, BiFeO3 (BFO) where multiferroicity coexist at room temperature. In this work, the Fe-Fe exchange interaction effects on the optical properties of BiFeO3 are analyzed by using both, linear and non linear spectroscopy as a function of temperature. Two and three magnons Raman scattering as well as detectable electromagnons in the second harmonic generation (SHG) signal are reported. Temperature studies up to 750 K reveals a cascade of phase transitions associated to different dynamic reorientations in the magnetic subsystem. These transitions were detectable by several optical methods including linear absorption, Raman spectroscopy and SHG due to the strong electric dipole coupling found between electromagnetic radiation and spin waves in BFO.

8:24AM H12.00003 Temperature studies of multiferroic TbMnO3 with resonant Raman scattering, ILKA MAHNS, M. BASTJAN, B. SCHULZ, S. MUELLER, A. RUSYDI, M. RUEBHAUSEN, IAP, University of Hamburg, Germany, N. ALIOUANE, D.N. ARCYRIOU, HMI, Berlin, Germany, H. BARATH, M. KIM, S.L. COOPER, Dept. of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Illinois — Using temperature dependent resonant Raman scattering with different excitation energies from the ultraviolet (UV) to near infrared (NIR), we have investigated the complex interplay between the orbital, structural and magnetic ordering in the multiferroic material TbMnO3. Depending on the scattering temperature at the Néel temperature at 41 K or the ferroelectric transition at T_F = 28 K is observed. In resonance studies with an incident frequency of 1.91 eV, the Jahn-Teller mode shows a strong softening below T_N. In the low frequency spectra, a quasielastic response is identified. The results give information about the electron-phonon coupling and the correlations between electronic and structural degrees of freedom that contribute to the multiferroic behavior in TbMnO3.

8:36AM H12.00004 Temperature- and field-dependent inelastic light scattering studies of TbMnO3, HARINI BARATH, MINJUNG KIM, S.L. COOPER, Dept. of Physics and Frederick Seitz Materials Research Laboratory, Univ. of Ill., Urbana-Champaign, M. RUEBHAUSEN, Institut fur Angewandte Physik, Universitat Hamburg, Hamburg, Germany, D.N. ARCYRIOU, Hahn-Meitner Institut, Berlin, Germany — TbMnO3 is one of several multiferroic materials that have coexisting magnetic and electric orders that are strongly coupled. Because it is exquisitely sensitive both to structural order and magnetic degrees of freedom, field-dependent inelastic light scattering measurements are ideally suited to studying magnetoelectric coupling and multiferroic phases in materials such as TbMnO3. By carefully examining the temperature- and field-dependent evolution of new magneto-elastic modes in various phases of TbMnO3, our study reveals several new features of the IC-C transition in TbMnO3, including the co-existence of distinct structural phases in the intermediate field regime around the IC-C phase transition and evidence for dynamical fluctuations of the IC and C phases outside the established phase boundaries.

1This work was supported by the Department of Energy under Grant No. DE-FG02-07ER46453. MR was supported by the German funding agency under RU 773/3-1.
8:48AM H12.00005 Pressure tuned phonon mode splitting in magnetic frustrated spinel ZnCr$_2$O$_4$, TAO ZHOU, ZHEN QIN, New Jersey Institute of Technology, ZHENXIAN LIU, Brookhaven National Lab, CHENGLIN ZHANG, SANG-WOOK CHEONG, Rutgers University — ZnCr$_2$O$_4$ has cubic spinel structure. Below 390 K, the geometrically frustrated magnet enters a paramagnetic state. Below 12.5 K, it undergoes a first-order phase transitions, resulting into an antiferromagnetic order and a structural distortion simultaneously. An IR-active phonon related to the Cr$^{3+}$ ion's motion undergoes a splitting at 12.5 K. This transition is explained as a spin-Peierls like transition. However, the exact cause and effect in such a transition is not clear. Is it because the lattice undergoes transition first, spin just follows, or is it spins' interaction that forces the lattice to undergo changes? Pressure can provide a crucial service in clarifying this issue, since pressure can change spin and lattice interactions in different ways, it can differentiate these two scenarios. We have measured the infrared absorption spectra of ZnCr$_2$O$_4$ under pressure. Our data shows that Tc, at which the spin-Peiers like transition occurs and the phonon at about 370 cm$^{-1}$ starts to show the splitting, increases from its ambient pressure value of 12.5 K to about 15.8 K at 1 GPa. This provides an important clue for the exact nature of this transition.

9:00AM H12.00006 Calculation of the Order Parameter and the Damping Constant in the Ferroelectric Phase for NaNO$_2$, ALI KIRACI, HUSEYIN KARACALLI, Abant Izzet Baysal University, HAMIT YURTSEVEN, Middle East Technical University — The temperature dependence of the order parameter and the damping constant is calculated in the ferroelectric phase in the range of 27 to 162 °C close to the phase transition (T$_{C}$=436 K) for NaNO$_2$. The values of the order parameter calculated from the molecular field theory, are used to evaluate the damping constant as a function of temperature on the basis of the soft phonon-hard phonon coupling model for NaNO$_2$ in the ferroelectric phase. By representing the damping constant calculated at various temperatures in terms of an Arrhenius plot, the activation energy is computed for this crystal in the ferroelectric phase. Our calculated order parameter agrees with the measured one and also the damping constant predicts the critical behaviour exhibited by the NaNO$_2$ crystal near the transition temperature in the ferroelectric phase. From the values of the activation energies obtained here, the mechanism of an order-disorder transition which involves the orientation of the NO$_2^−$ ions is investigated for NaNO$_2$.

9:12AM H12.00007 Pressure Dependence of the Phonon Modes of Hexagonal-RMnO$_3$¹, PENG GAO, TREvor A. TYSOn, Physics Department, New Jersey Institute of Technology, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, SUNG BAEK KIM, SANG-WOOK CHEONG, Dept. of Physics and Astronomy, Rutgers University — We present high pressure IR measurements of the phonon spectra of HoMnO$_3$ and YMnO$_3$. Measurements were conducted under the pressure range ambient to ~20 GPa. No phase changes were observed over this broad range of hydrostatic pressures. A strong non-linear variation of frequency with pressure is observed suggesting saturation at higher pressures. A discussion of the effect of hydrostatic pressure on the ferroelectric properties of these systems will be given based on comparisons with density functional calculations.

¹This work is supported by DOE Grant DE-FG02-07ER46402.

9:24AM H12.00008 Probing Spin-Lattice Correlations in Hexagonal RMnO$_3$ Multiferroics¹, TREvor TYSOn, ZHIQIANG CHEN, New Jersey Institute of Technology, SUNGBACK KIM, SANG-WOOK CHEONG, Rutgers University — The hexagonal multiferroic system RMnO$_3$ is known to exhibit strong spin-lattice correlations based on bulk thermal expansion measurements. Enhanced correlations at the spin ordering temperatures are observed. In this work, we examine the local structure about the R and Mn sites in order to determine the changes in atomic interactions which coincide with the spin alignments. Measurements over a broad range of temperatures are presented and estimates of the changes in atomic bond distances are given.

¹This work is supported by DOE Grant DE-FG02-07ER46402.

9:36AM H12.00009 Giant magneto-elastic coupling in multiferroic hexagonal manganites, SEONGSU LEE, Rutgers University, USA, A. PIROGOV, M.S. KANG, K.-H. JANG, SungKyunKwan University, Korea, M. YONEMURA, T. KAMIYAMA, KEK, Japan, S.-W. CHEONG, Rutgers University, USA, F. GOZZO, Paul Scherrer Institut, Switzerland, NAMSU SHIN, Pohang Accelerator Laboratory, Korea, H. KIMURA, Y. NODA, Tohoku University, Japan). J.-G. PARK, SungKyunKwan University, Korea — In order to investigate a possible structural change of RMnO$_3$ at the magnetic transition temperature, we have carried out high-resolution structural studies using neutron diffraction. Here we show that the hexagonal manganites RMnO$_3$ undergo an isostructural transition at T$_N$ with unusually large atomic displacements: two orders of magnitude larger than those seen in any other ordinary materials, resulting in a uniquely strong magneto-elastic coupling. For the first time, we could follow the exact atomic displacements of all the atoms in the unit cell as a function of temperature and found consistency with theoretical predictions based on group theories. We argue that this gigantic magneto-elastic coupling of RMnO$_3$ arises from geometrical frustration, and holds the key to the recently observed magnetoelectric phenomenon in this intriguing class of materials.

9:48AM H12.00010 Anomalous low-temperature magnetic ordering and spin-phonon coupling in BiFeO$_3$ thin films, MANOJ SINGH, Department of Physics and Institute of Functional Nano Materials, University of Puerto Rico, PR, USA, RAM KATIYAR, Department of Physics and Institute of Functional Nano Materials, University of Puerto Rico, PR, USA, W. PRELLIER, Laboratoire CRISMAT, CNRS, ENSICAEN, Caen Cedex, France, H.M. JANG, Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang, Korea, W. PRELLIER COLLABORATION, H. M. JANG COLLABORATION, RAM S. KATIYAR TEAM — Low-temperature magnetic properties and Raman spectra of epitaxial BiFeO$_3$ (BFO) thin films grown on (111) SrTiO$_3$ substrates have been studied. Zero-field-cooled (ZFC) and field-cooled (FC) magnetization curves showed a large discrepancy beginning at a characteristic temperature which did depend on the magnetic-field strength, suggesting a spin-glass-like behavior of the epitaxial BFO film with R3c symmetry. For all three major A$_1$-symmetry Raman modes (138, 170, and 214 cm$^{-1}$), there was a good linear correlation between the mode-frequency softening and the square of the in-plane magnetization in the temperature range between 80 and 300 K. These observations were ascribed to the spin-phonon coupling below the Néel temperature (T$_N$ = 643 K).

10:00AM H12.00011 Magneto-dielectric study of multiferroicity in biferroic YCrO$_3$, RELJA VASIC, HAI Song D. ZHOU, CHRIS R. WIEBE, JAMES S. BROOKS, Florida State University — Magneto-dielectric measurements are used to characterize multiferroicity in the doped monoclinic ferroelectric oxides Y$_{1−x}$Ca$_x$MnO$_3$ (x = 0, 0.15, 0.3). The focus of this study is on the effects of the magnetic field and Ca doping on the temperature- magnetic field dependent dielectric response of polycrystalline samples of rare earth chromates YCrO$_3$. YCrO$_3$ shows dielectric relaxation around 150 K related to the weak ferromagnetic ordering in system. Dipolar response is activated following Arrhenius formalism in the frequency range of 0.01-100 kHz, but it is independent on magnitude of magnetic field. As frequency increases dielectric peaks become broader and smaller. Dielectric constant relaxation behavior and magnetic phase transitions are not coupled through lattice distortions in this ferroelectric ferromagnetic system. YCrO$_3$ is an example of system with dipolar response in magnetic field without coupling with magnetic structure. There is strong dispersion of Debye relaxation peaks but absence of influence of magnetic field on ferroelectric system YCrO$_3$.
10:12AM H12.00012 Multiferroicity in the spin-1/2 quantum matter of LiCu$_2$O$_2$, ANDRIVO RUSYDI, ILKA MAHNS, SONJA MUELLER, MICHAEL RUEBHAUSEN, University of Hamburg, S. PARK, Y.J. CHOI, C.L. ZHANG, S.-W. CHEONG, Rutgers University, SERBAN SMADIC, PETER ABBAMONTE, UIUC, MARTIN VON ZIMMERMANN, DESY, GEORGE SAWATZKY, University of British Columbia — Multiferroicity in LiCu$_2$O$_2$ single crystals is studied using resonant soft x-ray magnetic scattering, hard x-ray diffraction, heat capacity, magnetic susceptibility, and electrical polarization. Two magnetic transitions are found at 24.6 K ($T_1$) and 23.2 K ($T_2$). Our data are consistent with a sinusoidal spin structure at $T_2 < T < T_1$ and with a helicoidal spin structure at $T < T_2$ giving rise to ferroelectricity. Surprisingly, above $T_2$ the correlation lengths of the spin structures increase as the temperature increases with dramatic changes of ~42% occurring along the c-axis. Our results demonstrate the intimate connection between frustration and coupling between electronic and magnetic polarizations in LiCu$_2$O$_2$.

10:24AM H12.00013 Magnetically-induced ferroelectric polarization in a molecule-based quantum magnet, VIVIEN ZAPF, FREDERIK FABRIS, National High Magnetic Field Lab, Los Alamos National Lab, MICHEL KENZELMANN, Laboratory for Solid State Physics, ETH Hönggerberg, Zurich, FEDOR BALAKIREV, NHMFL-LANL, YING CHEN, COLIN BROHOLM, Dept of Physics and Astronomy, Johns Hopkins University — Ferroelectricity coupled to antiferromagnetic (AFM) order has been observed in the organic S=1/2 chain compound CDC (CuCl$_2$ 2(CH$_3$)$_2$SO). For magnetic fields along the orthorhombic a-axis, AFM order occurs below $T_X$ = 0.93 K and $H \sim 4$ T. A spin-flop transition above $H_{sf} = 0.35$ T leads to a magnetically ordered state that breaks inversion symmetry along the b-axis for 0.35 T $< H < 4$ T. Measurements of the pyroelectric effect and the dielectric constant along both indicate ferroelectricity occurring in this same region of HT phase space with the spin polarization closely tracking the magnetic order parameter. A single quantum spin flop can be induced by successive field sweeps in the same direction. While the magnetically-induced ferroelectricity in CDC is far from practical temperatures and fields, it nevertheless demonstrates that this phenomenon can occur in a whole new class of compounds.

10:36AM H12.00014 Spin Dynamics and Spin-flop transition in Magnetoelastic Effect LiMnPO$_4$, J. LI, NCNR, National Institute of Standards and Technology; Dept. Material Science and Engineering, University of Maryland, W. TIAN, Ames laboratory and Dept. of Physics and Astronomy, Iowa State University, Y. CHEN, NCNR, National Institute of Standards and Technology; Dept. Material Science and Engineering, University of Maryland, J.L. ZARESTKY, D. VAKNIN, Ames laboratory and Dept. of Physics and Astronomy, Iowa State University, J.W. LYNN, NCNR, National Institute of Standards and Technology — Neutron scattering techniques were used to study the magnetic phase transition and spin dynamics in single crystal LiMnPO$_4$ both with and without magnetic field. Elastic scattering confirmed that LiMnPO$_4$ has a collinear antiferromagnetic ground state with moments along a-axis in zero-field. The temperature dependent order parameter, calculated from the integrated intensity of the (010) magnetic reflection, was fit to a power law equation, yielding a transition temperature $T_X = 33.8$ K. By applying magnetic field along the a-axis, the moments rotate from a-axis to the c-axis at a critical field of 3.5 Tesla at 5 K. The field dependent (100) and (001) intensities indicate a complicated intermediate state between the ground state and the spin-flop state. The critical field increased from 3.5 Tesla at 5 K to 4.5 Tesla near the transition, $T_X$. Spin-wave dispersion curves along the three principal axes were measured in the antiferromagnetic state at 4.5 K in zero magnetic field and were analyzed using a 3D Heisenberg model.

10:48AM H12.00015 Magnetic Excitations in LiCoPO$_4$, WEI TIAN, Ames laboratory and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, JIYING LI, JEFF LYNN, NCNR, National Institute of Standards and Technology, Gaithersburg, MD 20899, JEREL ZARESTKY, DAVID VAKNIN, Ames laboratory and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011 — LiCoPO$_4$ continues to attract much attention due to its exceptionally large magnetoelastic (ME) effect coefficient and the observed weak ferromagnetism and ME “butterfly loop” anomaly. To gain insight into the microscopic magnetic interactions in LiCoPO$_4$, inelastic neutron scattering experiments were performed in the antiferromagnetic phase at $T = 8$ K ($T_X \approx 21.8$ K). Weak dispersion was detected in the magnetic excitation spectra along the three crystallographic axes measured around the (0 1 0) magnetic reflection. A gap of ~4 Tesla was observed below $T_X$ that vanished above $T_X$. The peak energy was fit with a linear spin-wave approximation by explicitly including single-ion anisotropy terms in the Heisenberg spin Hamiltonian. The magnitude of the single-ion anisotropy is found to be comparable to the strongest nearest-neighbor magnetic interaction suggesting that the Co$^{2+}$ single ion anisotropy plays an important role in the spin dynamics of LiCoPO$_4$.

Tuesday, March 11, 2008 8:00AM - 10:36AM
Session H13 DCOMP GSCCM: Focus Session: Simulations of Matter at Extreme Conditions III: Classical MD, Potentials, and Energetic Materials Morial Convention Center 204

8:00AM H13.00001 Theoretical Approach for Developing Accurate Potentials for Molecular Dynamics Simulations: Thermoelastic Response of Aluminum, J.M. WINEY, Wash. State Univ., A. KUBOTA, Lawrence Livermore Nat. Lab., Y.M. GUPTA, Wash. State Univ. — To achieve the correct thermoelastic response of solids in classical simulations, a new approach is presented for developing accurate interatomic potentials. In this approach, the potentials are fitted to values for the atomic volume and the second and third-order elastic constants at $T = 0$K by extrapolating the room temperature values, using classical thermo-mechanical relations. This procedure avoids the low-temperature quantum regime, enabling recovery of the correct response in classical simulations to higher temperature. As an example of this approach, an EAM potential was developed for aluminum. Results using this potential provide consistently better agreement with thermoelastic data at higher temperature compared to previous EAM potentials. Our approach is applicable to the development of other types of potentials as well and is amenable to incorporating the results of first principles calculations performed using the classically extrapolated volume for $T = 0$K. Work supported by DOE.

8:12AM H13.00002 Petaflop simulations of shock-induced particulate ejection from copper, TIMOTHY C. GERMANN, JAMES E. HAMMERBERG, GUY DIMONTE, Los Alamos National Laboratory — We present the results of several large-scale, Non-Equilibrium Molecular Dynamics (NEMD) simulations of shock-induced surface instability development. We consider single crystal Cu described by an embedded atom method (EAM) potential and driven by a shock wave along the [111] crystallographic direction, impinging upon a roughened Cu/vacuum or Cu/Ne interface. The initial temperature is 300K and the NEMD simulation cell is a quasi-2D 2.23µm × 5.67µm slab geometry, 1.5 nm thick in the (periodic) third dimension. The first third of the sample length (1.89µm) is occupied by Cu (5.3 × 10$^8$ atoms), and the remainder either empty vacuum or Ne gas at a pressure of 0.67 MPa (1.95 × 10$^8$ atoms). The Cu/Ne (or Cu/vacuum) interface has an initial perturbation with average amplitude 30 nm and dominant wavelength of 0.74µm. A shock wave is created by driving the free end of the Cu slab at a fixed particle velocity $u_p = 2.0$ to 3.5 km/s. Single-mode and multi-mode simulations were considered using 212,992 CPUs of the LLNL BlueGene/L supercomputer for times approaching 1 ns. At the higher particle velocities, the Cu release state is in the fluid-solid mixed phase. We discuss the evolution of the density and velocity distributions of the ejected mass, the modes of particle breakup, and comparisons to source theories of ejecta formation and Richtmyer-Meshkov instabilities.
8:24AM H13.00003 Interatomic bond-order potentials for molecular dynamics simulations of materials at extreme conditions. ROMAIN PERRIOT, MIKALAI BUDZEVICH, IVAN OLEYNIK, University of South Florida — Molecular dynamics (MD) is a powerful research tool for studying materials at extreme conditions. At the heart of MD are the interatomic potentials, whose quality in describing a variety of chemical effects, including bond-breaking and bond-making, plays a decisive role in delivering meaningful results. We have performed extensive MD simulations of shock compression of covalently bonded materials, such as diamond and silicon, and found that REBO interatomic potential for diamond and EDIP potential for Si have substantial deficiencies at large pressures and temperatures in spite of the fact that the near equilibrium properties of both diamond and silicon are well reproduced. We are addressing this outstanding issue by developing analytic bond-order potentials (BOPs) specifically for the simulation of covalently bonded materials at extreme conditions. These BOPs include explicit analytic expressions for both the $\sigma$ and $\pi$ bonds. We will discuss important steps of BOP construction which includes devising a first-principle database of fundamental materials properties, fitting this database by the orthogonal tight-binding, and devising the analytic BOPs using the direct link between TB and analytic BOPs via the bond orders.

8:36AM H13.00004 Interatomic Potentials for Large-Scale Simulations of High-Pressure, High-Temperature Phenomena, RAMON RAVELO, University of Texas at El Paso; Applied Physics Division, Los Alamos National Laboratory — The use of large-scale atomistic simulations in the study of high-compression, high strain-rate phenomena has dramatically increased in the last decade. Most of this type of simulations utilize classical empirical or semi-empirical potentials to describe the inter-atomic interactions. The regime of validity of most of these potentials is however often limited to a narrow region of the pressure-temperature phase diagram. In the development of accurate inter-atomic potentials for material simulations at high-pressures or temperatures, a high degree of transferability is desirable without resorting to fitting everywhere in phase space. We will review two popular cluster functional models: the embedded-atom-method (EAM) and the modified embedded-atom-method (MEAM). The embedded atom method provides a very good description of metallic properties at a low computational cost and has become the workhorse of large-scale atomistic simulations of metallic systems. The modified embedded-atom-method is an improvement of EAM which includes the effect of angular bonding. We outline inherent limitations of these models and present a systematic approach to improving their transferability and predictive accuracy at high pressures and/or temperatures.

9:12AM H13.00005 Ultrafast semi-metallic layer formation in detonating nitromethane, EVAN REED, M. RIAD MANAA, LAURENCE FRIED, KURT GLAESERMANN, Lawrence Livermore National Laboratory, JOHN JOANNOPOLOS, Massachusetts Institute of Technology — We present the first quantum molecular dynamics simulations behind a detonation front (up to 0.2 ns) of the explosive nitromethane (CH$_3$NO$_2$) represented by the density-functional-based tight-binding method (DFTB). This simulation is enabled by our recently developed multi-scale shock wave molecular dynamics technique (MSST) that opens the door to longer duration simulations by several orders of magnitude. The electronic density of states around the Fermi energy initially increases as metastable material states are produced but then later decreases, perhaps unexpectedly. These changes indicate that the shock front is characterized by an increase in optical thickness and conductivity followed by a reduction around 100 picoseconds behind the front. We find that a significant population of intermediate metastable molecules are charged and charged species play an important role in the density of states evolution. The transient transformation to a semi-metallic state can be understood within the Anderson picture of metalization.

9:24AM H13.00006 Reactive Molecular Dynamics Studies of Thermal Induced Chemistry in HMX, JASON QUENNEVILLE, TIMOTHY GERMANN, THOMAS SEWELL, EDWARD KOBEN, Los Alamos National Laboratory — Equilibrium molecular dynamics (MD) simulation of high explosives can provide important information on their thermal decomposition by helping to characterize processes with timescales that are much longer than those attainable with non-equilibrium MD shock studies. A reactive force field is used with MD to probe the chemistry induced by intense heating (‘cook-off’) of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). The force field (ReaxFF) was developed by van Duin, Goddard and coworkers at CalTech and has shown promise in predicting the chemistry in a variety of systems, including RDX and TATB under either shock compression or intense heat. In the current work, we investigate the effect of initial equilibration temperature (1000 to 1500 K), volumetric compression, crystal polymorph ($\beta$ and $\delta$), and system size (ranging from 150 to 1200 molecules) on the reaction rate and reaction products. Finally, we will compare these results with those from our previous work on TATB. A C. T. Van Duin, et al., J. Phys. Chem. A, 1005, 9396 (2001).

9:36AM H13.00007 Anisotropic Constitutive Relationships in Energetic Materials: TATB, MIKALAI M. BUDZEVICH, AARON LANDERVILLE, MIKE CONROY, IVAN I. OLEYNIK, University of South Florida, CARTER T. WHITE, Naval Research Laboratory — One of the principal thrusts in energetic materials (EM) research is the acquisition of accurate equations of state (EOS) for various important classes of EMs. In the past, both theoretical and experimental studies concentrated on hydrostatic EOS. However, these isotropic EOS still need to be expanded to include anisotropic materials response, including uniaxial compression which are more relevant to shock initiation of detonation. To this end, we performed first-principles density functional calculations of the EOS for TATB, including uniaxial compressions in the [100], [010], [001], [110], [101], and [111] crystallographic directions. Equilibrium properties, such as lattice parameters and elastic constants, as well as the hydrostatic EOS were calculated and compared with experimental results. Finally, we discuss the possible relationship between shear stresses induced by the uniaxial compression of TATB and the relative shock sensitivities of different crystallographic directions.

9:48AM H13.00008 First-Principles Reactive Molecular Dynamics of Chemistry in Detonating Energetic Materials, AARON LANDERVILLE, IVAN I. OLEYNIK, University of South Florida, MORTKO A. KOZHUSHNER, Russian Academy of Sciences, CARTER T. WHITE, Naval Research Laboratory — We investigated the initial chemistry of shock compressed energetic materials that results from inter-molecular collisions behind the shock wave front by performing first-principles MD simulations of bimolecular collisions for PETN and RDX with different crystallographic orientations and velocities. For each orientation, we determined the threshold collision velocity for reaction, the reaction timescales, and the products of decomposition. We find that the calculated threshold velocities lie within the range of typical particle flow velocities in detonating materials. Owing to the extremely short reaction timescales ($\sim 10^{-14}$s), these initial chemical events are largely driven by the direct collision dynamics, instead of temperature.
10:00AM H13.00009 Reactive MD simulations of anisotropic response of PETN under high-rate shear deformation1. XU PENG, SERGEY ZYBIN, California Institute of Technology; AIDAN P. THOMPSON, Sandia National Lab; WILLIAM A. GODDARD, California Institute of Technology — Several experiments have indicated that the shock sensitivity of single crystal energetic materials can depend on the crystallographic direction. We develop a compress-and-shear modeling approach to study the mechanisms of anisotropic shock sensitivity using the ReaxFF reactive molecular dynamics. ReaxFF is a first-principles based force field capable to reproduce the quantum chemical energies of the reactants, intermediates and transition states with functional forms suitable for large-scale molecular dynamics simulations of chemical reactions under extreme conditions. In this presentation we will discuss the results of high-rate shear simulations of uniaxially compressed PETN. We found noticeable differences in the physical and chemical responses of PETN for different combinations of the slip system and compression direction. The simulation results agree well with the experimental shock-initiation sensitivity data and Dick’s steric hindrance theory.

Supported by DoD/ARO (W911NF-05-1-0345) and DoD/ONR (N00014-05-1-0778)

10:12AM H13.0009 First-Principles Constitutive Relationships in PETN and HMX under Hydrostatic and Uniaxial Compressions1. SERGEY V. ZYBIN, California Institute of Technology, MICHAEL W. CONROY, IVAN I. ÖYLENIK, University of South Florida, CARTER T. WHITE, Naval Research Laboratory — The physical mechanisms leading to shock-induced detonation at the atomic level are ultimately related to energetic materials response to uniaxial compression at the shock front. Due to the intrinsic anisotropy of the constitutive relationships, a description of the compressed state should be extended beyond hydrostatic equations of state that are frequently used for analysis of precursor states of EMs. In this presentation, we will discuss the results of first-principles density functional theory calculations of both hydrostatic and uniaxial compressions in the [100], [010], [001], [110], [101], [011], and [111] directions applied to the energetic materials PETN-I and β-HMX. A comparison will be made of available experimental data with calculated physical properties such as unit cell geometry, isothermal equations of state, and elastic constants. The presentation will focus on the anisotropic nature of the constitutive relationships in molecular crystals under uniaxial compression. The behavior of the shear stress projections on available slip systems upon uniaxial strain and their possible relationship to experimental shock-initiation sensitivity data will be discussed.

Supported by DoD/ARO and DoD/ONR

10:24AM H13.00011 Reactive molecular dynamics simulations of shocked PETN2. JOANNE BUDZIEN, AIDAN P. THOMPSON, Sandia National Laboratories, SERGEY V. ZYBIN, California Institute of Technology — We have performed molecular dynamics simulations of PETN crystals subjected to shock along the [100] direction. Using the reactive forcefield, ReaxFF, and the molecular dynamics code, GRASP, allows us to track the chemical reactions that occur as both a function of time and position. By simulating larger systems, we can observe the formation of both primary and secondary products to make comparisons with experiments. Composition profiles of these products will be shown along with profiles of stress, temperature, and potential energy.

Supported by DoD/ARO (W911NF-05-1-0345) and DoD/ONR (N00014-05-1-0778)

Tuesday, March 11, 2008 8:00AM - 10:48AM — Session H14 DAMOP: Cold Gases: One Dimensional Phenomena Morial Convention Center 205

8:00AM H14.00001 Feshbach physics in a one-dimensional optical lattice, NICOLAI NYGAARD, RUNE PIIL, KLAUS MØLMER, Lundbeck Foundation Theoretical Center for Quantum System Research, Department of Physics and Astronomy, University of Aarhus — We consider a pair of atoms in a one-dimensional optical lattice interacting via a Feshbach resonance. Using a two-channel description of the resonance, we derive the analytic form of the Fano scattering resonance inside the continuum band and the discrete bound states outside the band. We suggest experiments to probe and utilize the special properties of the system, which arise from the continuum having an upper edge.

8:12AM H14.00002 Pairing states of a polarized Fermi gas trapped in a one-dimensional optical lattice, ADRIAN FEIGUIN, University of Maryland, College Park, and Microsoft Station Q, FABIAN HEIDRICH-MEISNER, Institut für Theoretische Physik C, RWTH Aachen, Germany — We study the properties of a one-dimensional (1D) gas of fermions trapped in a lattice by means of the density matrix renormalization group method, focusing on the case of unequal spin populations, and strong attractive interaction. In the low density regime, the system phase-separates into a well defined superconducting core and a fully polarized metallic cloud surrounding it. We argue that the superconducting phase corresponds to a 1D analogue of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, with a quasi-condensate of tightly bound bosonic pairs with a finite center-of-mass momentum that scales linearly with the magnetization. In the large density limit, the system allows for four phases: in the core, we either find a Fock state of localized pairs or a metallic shell with free spin-down fermions moving in a fully filled background of spin-up fermions. As the magnetization increases, the Fock state disappears to give room for a metallic phase, with a partially polarized superconducting FFLO shell and a fully polarized metallic cloud surrounding the core.

8:24AM H14.00003 The FFLO Phase in Imbalanced Spin Fermions in 1-d1. MIRIAM HUNTLEY, MIT, RICHARD SCALETTAR, UC Davis, GEORGE BATROUNI, Université de Nice-Sophia Antipolis, VALERY ROSSEAU, Universiteit Leiden Instituut Lorentz — Pairing in imbalanced spin populations has lately been the focus of many experimental and theoretical studies. Different mechanisms have been proposed to explain how pairing takes place between the two fermionic species. In this talk we will present exact Quantum Monte Carlo simulations of imbalanced spin populations in one dimension. We will first discuss the case where no confining potential is imposed. Here we have found that the pair-pair correlation function develops oscillations at nonzero polarizations, corresponding to a pair momentum distribution that, instead of being peaked at zero, is peaked at a momentum equal to the difference in the Fermi momenta. This indicates that the pairing mechanism is described by the Fulde Ferrel Larkin Ovchinnikov (FFLO) picture, and not by other proposed phases which require zero-momentum pairing. When a confining potential is included in the simulations, we find that the FFLO oscillations are still present. In addition, we show that the local polarization displays a dip in the center of the trap, similar to experimental observations performed with 3-dimensional optical traps.

1Supported by NSF PHY-0649297 (REU), RTS by DARPA/AFOSR, GGB by the CNRS (France) PICS 18796, and VGR by the research program of the ‘Stichting voor Fundamenteel Onderzoek der Materie (FOM)’. 

3MHH is supported by NSF PHY-0649297 (REU), RTS by DARPA/AFOSR, GGB by the CNRS (France) PICS 18796, and VGR by the research program of the ‘Stichting voor Fundamenteel Onderzoek der Materie (FOM)’. 
8:36AM H14.00004 One dimensional trapped fermions with attractive contact interactions

MICHELE CASULA, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana-Champaign — Recent advances in cold atomic physics allow creation of optical lattices which reproduce well defined model Hamiltonians. This opens the route to resolve the phases of strongly correlated systems by carrying out experiments with trapped cold atoms. In this work, we study the properties of one dimensional trapped spin 1/2 fermions with attractive contact interactions by means of exact quantum Monte Carlo techniques. According to the local density approximation (LDA), such a system is expected to show phase separation between a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state and either fully polarized or fully paired outer shells.[1] Here we show how the size and temperature affect the LDA phase boundaries. Mapping out the dependence on the number of particles, temperature, and interaction strength is extremely useful to benchmark experiments where cold atoms are trapped in arrays of cigar-shaped tubes, and understand whether the related setup will be able to detect the signatures of the FFLO state.


3We acknowledge support from the DARPA grant W911NF-07-1-0464 and the computer facilities at NCSA.

8:48AM H14.00005 Quantum Monte Carlo study of the visibility of one-dimensional Bose-Fermi mixtures

CHRISTOPHER VARNEY, University of California, Davis, VALERY ROUSSEAU, Institut Lorentz, RICHARD SCALETTAR, University of California, Davis — The study of ultra-cold, optically trapped atoms has opened new vistas in the physics of correlated quantum systems. Much attention has now turned to mixtures of bosonic and fermionic atoms. A central puzzle is the disagreement between the experimental observation of a reduced bosonic visibility \( V_b \), and quantum Monte Carlo (QMC) calculations which show \( V_b \) increasing. In this talk, we present new QMC simulations which evaluate the density profiles and \( V_b \) of mixtures of bosons and fermions in one-dimensional optical lattices. We resolve the discrepancy between theory and experiment by identifying parameter regimes where \( V_b \) is reduced, and where it is increased. We present a simple qualitative picture of the different response to the fermion admixture in terms of the superfluid and Mott insulating domains before and after the fermions are included. Finally, we show that \( V_b \) exhibits kinks which are tied to the domain evolution present in the pure case, and also additional structure arising from the formation of composite boson-fermion particles.

9:00AM H14.00006 Molecular superfluid phase in one-dimensional multicomponent fermionic cold atom systems

GUILLAUME ROUX, LPT, IRSAMC, CNRS, Universite Paul Sabatier, Toulouse, France and Institut fur theorethische Physik C, RWTH Aachen, SYLVAIN CAPPONI, LPT, IRSAMC, CNRS, Universite Paul Sabatier, Toulouse, France, PHILIPPE LECHEMONNANT, LPTMC, Universite Pierre et Marie Curie, CNRS, Paris, France, EDOUARD BOULAT, LMPQ, Universite Paris Diderot - Paris 7, CNRS, France, STEVEN R. WHITE, Department of Physics and Astronomy, University of California, Irvine, USA — We study a simple model of \( N \)-component fermions with contact interactions which describes fermionic atoms with \( N = 2F + 1 \) hyperfine states loaded into a one-dimensional optical lattice. We show by means of analytical and numerical approaches that, for attractive interaction, a quasi-long-range molecular superfluid phase emerges at low density. In such a phase, the pairing instability is strongly suppressed and the leading instability is formed from bound-states made of \( N \) fermions.

1Support of the NSF under Grant DMR-0605444.

9:12AM H14.00007 Spin and charge velocities of one-dimensional boson-fermion mixture

SHIH-JIAN GU, Department of Physics and ITP, The Chinese University of Hong Kong, Hong Kong, China, JUNPENG CAO, Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, HAIO-QING LIN, Department of Physics and ITP, The Chinese University of Hong Kong, Hong Kong, China — We study the ground state and elementary excitations of a one-dimensional mixture of scalar bosons and spin-1/2 fermions with repulsive delta-function interaction by the Bethe-ansatz method. Though the ground state properties are dramatically changed once bosons are mixed into fermions, the spin and charge excitations still feature linear dispersions, and their velocities satisfy a simple universal relation.

2This work is partly supported by HKRGC of No. CUHK-401504, and NSFC under Grant No. 10574150.

9:24AM H14.00008 The ground state properties of two-component ultra-cold Fermi gas in hard wall confinement

BO-BO WEI, Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, NT, Hong Kong, China, JUN-PENG CAO, Institute of Physics and Laboratory of Condensed Matter Physics, The Chinese Academy of Sciences, China, SHI-JIAN GU, HAI-QING LIN, Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, NT, Hong Kong, China — We investigate the ground state properties of a one-dimensional two-component ultra-cold Fermi gas subjected to a hard wall trap. The explicit form of the wave function is obtained by solving the Bethe Ansatz equations numerically. Then we obtain the one-body density matrix of the system for different interaction strengths. Results of the momentum distribution of the atoms, which are obtained from the Fourier transform of the one-body density matrix, are reported for different interaction strengths. This interacting system may be experimentally accessible using ultra-cold atoms.

9:36AM H14.00009 Quantum Phase Transition between (Luttinger) Liquid and Gas of Cold Molecules

DIMA FELDMAN, KAM TUEN LAW, Brown University — We consider cold polar molecules confined in a helical optical lattice similar to those used in holographic microfabrication. An external electric field polarizes molecules along the axis of the helix. The large-distance inter-molecular dipolar interaction is attractive but the short-scale interaction is repulsive due to geometric constraints and thus prevents collapse. The interaction strength depends on the electric field. We show that a zero-temperature liquid-gas transition occurs at a critical field. It can be observed under experimentally accessible conditions.

1We acknowledge the support by NSF under Grant No. DMR-0544116

9:48AM H14.00010 Dynamics of excitations in a one-dimensional Bose liquid

MAXIM KHODAS, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, MICHAEL PUSTILNIK, School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA, ALEX KAMENEV, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, LEONID I. GLAZMAN, Department of Physics, Yale University, New Haven, Connecticut, USA, 06520 — We studied the dynamical structure factor \( S(q, \omega) \) of interacting bosons in one-dimension. The sharp resonant peak \( S(q, \omega) \propto \delta(\omega - \epsilon(q)) \) as predicted by the Bogolubov theory is transformed into a power law singularity, \( S(q, \omega) \propto (\omega - \epsilon(q))^{-\theta(q)} \) due to the strong quantum fluctuations. The corresponding momentum dependent exponent \( \mu(q) \) is evaluated using the Lieb-Liniger model. The full momentum dependence \( \mu(q) \) has been found in the strongly interaction regime using the Fermi Bose mapping. For the large momentum \( q \) the different method allows us to express the exponent through the Luttinger liquid parameters. The two results agree in their common region of applicability.

1Research in University of Minnesota is supported by DOE (Grant No. DE-FG02-06ER46310) and A. P. Sloan Foundation. Research in Georgia Tech is supported by NSF (Grant No. DMR-0604107).
scales as we analyze the dependence of the density of created excitations on the ramp rate $\delta$. We find that for strongly interacting commensurate bosons this density scales as $\sqrt{\delta}$, while for weakly interacting bosons it scales as $\delta^2$.

We compute experimentally relevant response functions and we derive asymptotically exact expressions near the quantum critical points separating the Haldane insulator from the conventional Mott and density wave insulators. In particular, we predict a narrow absorption peak in Bragg spectroscopy experiments, due to the excitation of a single domain wall in the string order.


10:24AM H14.0011 Bosonic Mixtures in one-dimensional optical lattices I., LUDWIG MATHEY, NIST, Gaithersburg, and JIQ, UMD, ANZI HU, JIQ, UMD, and NIST, Gaithersburg, IPPEI DANSHTA, JIQ, UMD, and Waseda University, Tokyo, CARL WILLIAMS, JIQ, UMD, and NIST, Gaithersburg, CHARLES CLARK, NIST, Gaithersburg, and JIQ, UMD — We study binary bosonic mixtures of ultra-cold atoms, confined to one dimension in an optical lattice, for various densities. Within a Luttinger liquid description, using renormalization group equations at second order, we determine both ordered and quasi-ordered phases of these mixtures. At commensurate filling, e.g., unit-filling and half-filling, we find different types of localized phases, whereas for densities that are incommensurate to the lattice, but equal for the two species, we find the behavior of a spin gap transition. We discuss the properties of the various phases, and how they could be detected in experiment.

Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H15 GQL: Focus Session: Superconducting Qubits I Morial Convention Center 207

8:00AM H15.00001 Designing quantum-information-processing superconducting qubit circuits that exhibit lasing and other atomic-physics-like phenomena on a chip\(^1\), FRANCO NORI, Frontier Research System, RIKEN, Saitama, Japan; and Physics Dept., Univ. of Michigan, Ann Arbor, USA. — Superconducting (SC) circuits can behave like atoms making transitions between a few energy levels. Such circuits can test quantum mechanics at macroscopic scales and be used to conduct atomic-physics experiments on a silicon chip. This talk overviews a few of our theoretical studies on SC circuits and quantum information processing (QIP) including: SC qubits for single photon generation and for lasing; controllable couplings among qubits; how to increase the coherence time of qubits using a capacitor in parallel to one of the qubit junctions; hybrid circuits involving both charge and flux qubits; testing Bell’s inequality in SC circuits; generation of GHZ states; quantum tomography in SC circuits; preparation of macroscopic quantum superposition states of a cavity field via coupling to a SC qubit; generation of nonclassical photon states using a SC qubit in a microcavity; scalable quantum computing with SC qubits, and information processing with SC qubits in a microwave field. Controllable couplings between qubits can be achieved either directly or indirectly. This can be done with and without coupler circuits, and with and without data-buses like EM fields in cavities (e.g., we will describe both the variable-frequency magnetic flux approach and also a generalized double-resonance approach that we introduced). It is also possible to “turn a quantum bug into a feature” by using microscopic defects as qubits, and the macroscopic junction as a controller of it. We have also studied ways to implement radically different approaches to QIP by using “cluster states” in SC circuits. For a general overview of this field, see, J.Q. You and F. Nori, Phys. Today 58 (11), 42 (2005)

\(^1\)Work supported by RIKEN, NSA, LPS, ARO, NSF, CREST, JSPS.

8:36AM H15.00002 A Tunable Coupling Architecture For Josephson Phase Qubits, RADOSLAW BIALCZAK, M. ANSMANN, M. HOFHEINZ, E. LUCERO, R. MCPHERSTON, M. NEELEY, A.Q. O’CONNELL, H. WANG, A. CLELAND, J. MARTINIS, U.C. Santa Barbara — Previous coupled-qubit experiments with Josephson phase qubits have used a fixed coupling scheme. However, in order to create high-fidelity multi-qubit gates, a tunable coupling scheme is needed. Fixed coupling schemes cannot be used because single-qubit operations on a coupled-qubit system cannot be performed with high fidelity due to the errors induced by always-on coupling. Fixed coupling also allows for crosstalk between coupled qubits during measurement. We show how to implement a tunable-coupling architecture for Josephson phase qubits using simple linear elements. This architecture can be used to vary the interaction strength from fully-off to fully-on allowing us to get around the problems inherent with the use of a fixed coupling scheme.

8:48AM H15.00003 High-fidelity gates in Josephson phase qubits, ERIK LUCERO, University of California at Santa Barbara, MARKUS ANSMANN, RADOSLAW BIALCZAK, MAX HOFHEINZ, NANDA KATZ, The Hebrew University of Jerusalem, MATTTHEW NEELEY, AARON O’CONNELL, HAOMIAO WANG, ANDREW CLELAND, JOHN MARTINIS — Complex algorithms for a quantum computer will require error correction, which calls for logic gates with fidelity below a fault tolerant threshold. We present significant progress towards this goal with our detailed measurements of gate fidelity. We carefully separate out gate and measurement error and construct a complete error budget to demonstrate single qubit gate fidelities of 0.98, limited by energy relaxation. We introduce a new metrology tool ‘a Ramsey interference error filter’ that can measure the excited two-state population down to $10^{-4}$, a magnitude near the fault tolerant threshold. This measurement demonstrates that our quantum system remains in the two-state qubit manifold during our single qubit operations. This precision and accuracy is made possible by custom control electronics that can create arbitrarily shaped microwave pulses.
9:00AM H15.00004 Recent progress towards violating the CHSH Bell inequality in Josephson phase qubits. MARKUS ANSGMANN, University of California at Santa Barbara, RADOUSŁAW BIALCZAK, MAX HOFHEINZ, NADAV KATZ, The Hebrew University of Jerusalem, ERIK LUCERO, MATTHEW NEELEY, AARON O’CONNELL, HAOHUA WANG, ANDREW CLELAND, JOHN MARTINIS — Improvements of gate fidelity and control electronics for Josephson phase qubits have provided the foundation for revisiting Bell’s inequality. The violation of Bell’s inequality is the primary argument against the possible existence of a hidden-variable-theory as an alternative to quantum mechanics. It also serves as a convincing demonstration that a given system behaves in a truly non-classical way. The most widely accepted form of Bell’s inequality follows closely along a correlation measurement proposed by Clauser, Horne, Shimony and Holt (CHSH) in 1969. Here we present our latest attempt to implement the CHSH Bell test using Josephson phase qubits. The nature of this experiment places high demands on the current state of the art in solid state qubits — on qubit performance measures such as the energy relaxation time $T_1$, the decoherence time $T_2$, single and two qubit gate fidelities, and measurement fidelities. We will examine these demands with respect to the number of fronts we have improved upon in our system.

9:12AM H15.00005 Analysis of Bell inequality violation in superconducting phase qubits$^1$. ABRAHAM G. KOFMAN, ALEXANDER N. KOROTKOV, University of California, Riverside — We analyze conditions for violation of the Bell inequalities, focusing on experiments with Josephson phase qubits. In the ideal case we discuss all possible situations of maximum violation, but mainly focus on two important types of optimal qubit-measurement directions in the pseudospin space, lying within either horizontal or vertical planes. Only the vertical type remains optimal in presence of local measurement errors, while in the case of local decoherence of qubits either the horizontal or vertical configuration is optimal. Besides local measurement errors and decoherence, we also discuss the effect of measurement crosstalk, which affects both the classical inequality and the quantum result. In particular, we propose a version of the Bell inequality which is insensitive to the crosstalk.

9:24AM H15.00006 High Fidelity Universal Quantum Gates in Superconducting Qubit Systems Using Non-adiabatic Rapid Passage. FRANK GAITAN, RAN LI, Southern Illinois University — Recent theoretical work$^2$ has suggested that a class of non-adiabatic rapid passage sweeps first realized experimentally in NMR systems in 1991, can be used to produce a high fidelity universal set of quantum gates. We show how this class of sweeps can be implemented in both superconducting charge and flux qubit systems. We discuss the current challenges facing the use of these sweeps to produce a universal set of high fidelity quantum gates in superconducting qubit systems.

$^1$Supported by the DTO/ARO grant

9:36AM H15.00007 Improving dc SQUID Phase Qubit Lifetimes through Increased Isolation from Bias Leads$^3$. ANTHONY PRZYBYSZ, TAUNO PALOMAKI, SUDEEP DUTTA, FRED WELLSTOOD, RUPERT LEWIS, HANHEE PAIK, HYEOKSHIN KWON, BEN COOPER, KAUSHIK MITRA, BOB ANDERSON, ALEX DRAGT, CHRIS LOBB, QJI, University of Maryland — The dc SQUID phase qubit has been plagued by a relatively short coherence time, $T_2$, and relaxation time, $T_1$ (tens of ns). By using a sapphire substrate and small (15 $\mu$m$^2$ or less) Al/AIO$_x$/Al junctions the performance of the qubit has improved to the point where the impedance of the bias leads is the main source of dissipation and decoherence in the device. We identify the main circuit parameters that effect the isolation (junction capacitance, loop inductance, etc.), and present designs to improve the qubits isolation from the bias leads.

$^3$This work was funded by the Joint Quantum Institute, the Center for Nanophysics and Advanced Materials, and the Department of Defense.

9:48AM H15.00008 Anomalous Avoided Level Crossings in a Cooper-Pair Box Spectrum$^4$. ZAEILL KIM, V. ZARETSKEY, Y. YOON, Department of Physics, University of Maryland, J.F. SCHNEIDERMAN, M.D. SHAW, Department of Physics and Astronomy, University of Southern California, P.M. ECHTERNACH, Jet Propulsion Laboratory, California Institute of Technology, F.C. WELLSTOOD, QJI, CNAM, Department of Physics, University of Maryland, B.S. PALMER, LPS — We have used a radio-frequency superconducting single-electron transistor to measure the detailed spectrum of an Al/AIO$_x$/Al Cooper-pair box (CPB) qubit. The CPB had a charging energy $E_C/k_B=0.58$ K and a Josephson energy $E_J/k_B$, which can be tuned by an external magnetic flux, between 0.1 and 1 K. From 15 to 50 GHz we have found four anomalous avoided level crossings in the excited state spectrum of the CPB. We note the splitting size has a strong dependence on the Josephson energy and the location of the splitting depends on the gate voltage of the CPB, evidence that the CPB is coupled to other quantum systems that are charged. We compare our results to a model Hamiltonian that describes a charge fluctuator coupled to a CPB and extract fit parameters that provide microscopic information about the charge fluctuators.

$^4$This research was supported by the National Security Agency.

10:00AM H15.00009 Detailed Study of the Excited State Lifetime of a Cooper-Pair Box$^5$. VITALEY ZARETSKEY, Z. KIM, Y. YOON, Department of Physics, UMD, J. F. SCHNEIDERMAN, M. D. SHAW, Department of Physics and Astronomy, USC, P. M. ECHTERNACH, JPL, Caltech, F. C. WELLSTOOD, QJI, CNAM, Department of Physics, UMD, B. S. PALMER, LPS — We have used a radio-frequency superconducting single-electron transistor (rf-SET) to measure the lifetime of the excited state ($T_1$) of an Al/AIO$_x$/Al Cooper-pair box (CPB) qubit with a charging energy $E_C/k_B=0.58$ K. We measured the lifetime by continuously measuring the decay of the qubit from a mixed state. By effectively decreasing $E_J/k_B$ from 1 K to 0.1 K we could increase $T_1$ from 50 ns to 5 s which indicates that charge is the dominant noise source. Additionally we noted that the decay rate as a function of transition frequency had several narrow peaks in the range 15 to 50 GHz. These peaks correlated with the locations of anomalous avoided level crossings we observed in the excited state spectrum of the CPB$^4$, suggesting that interaction with microstates is a source of dissipation for these qubits.

$^5$This research was supported by the NSA.

$^2$Anomalous Avoided Level Crossings in a Cooper-Pair Box Spectrum, ZAEILL KIM et al., BAPS (March 2008)
voltage. Measurements are performed using RF reflectometry to measure the quantum capacitance of each device.

We discuss the dependence of these rates on a variety of experimental parameters, such as RF power, microwave power, magnetic flux, sample temperature, and gate voltage. Measurements are performed using RF reflectometry to measure the quantum capacitance of each device.

10:24AM H15.00011 Robust optimal quantum gates for Josephson charge qubits, SIMONE MONTANGERO, NEST-CNR-INFM & Scuola Normale Superiore, P.zza dei Cavalieri 7, Pisa, Italy, TOMMASO CALARCO, ITAMP, Harvard University, Cambridge, MA 02138, U.S.A., ROSARIO FAZIO, NEST-CNR-INFM & Scuola Normale Superiore, P.zza dei Cavalieri 7, Pisa, Italy — Quantum optimal control theory allows us to design accurate quantum gates. We employ it to design high-fidelity two-bit gates for Josephson charge qubits in the presence of both leakage and noise. Our protocol considerably increases the fidelity of the gate and, more importantly, it is quite robust in the disruptive presence of 1/f noise. The improvement in the gate performances discussed in this work (errors ∼10^{-3}±10^{-4} in realistic cases) allows to cross the fault tolerance threshold.

10:36AM H15.00012 Suppression of decoherence due to classical noise by dynamical decoupling, LUKAZS CYWINSKI, ROMAN M. LUTCHYN, CODY P. NAVE, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute; Department of Physics; University of Maryland — We consider a pure dephasing model in the context of superconducting qubits. We show that the coherence time T2 can be significantly increased by the application of a series of π pulses. The most well known example, spin echo, a one pulse sequence, removes inhomogeneous broadening. However, T2 can be further increased by applying more pulses. We discuss the experimental implications of various pulse sequences in the context of classical 1/f noise in a Cooper-pair box qubit. We show that a recently proposed coherence-restoring pulse sequence [1, 2], discovered in the context of the spin-boson model, is optimal in certain regimes of parameter space. [1] G. S. Uhrig Phys. Rev. Lett. 98, 100504 (2007) [2] B. Lee, W. M. Witzel, S. Das Sarma, arXiv:0710.1416 (2007).

1This work is supported by the LPS-NSA-CMTC grant and by a fellowship from the Joint Quantum Institute (RL).

10:48AM H15.00013 The effect of dynamical decoupling in the case of a single fluctuator coupled to a qubit, CODY NAVE, ROMAN LUTCHYN, LUKAZS CYWINSKI, SANKAR DAS SARMA, Condensed Matter Theory Center and Joint Quantum Institute; Department of Physics; University of Maryland - College Park — We consider the role of dynamical decoupling in the case of a single classical fluctuator coupled to a qubit which is operated in a pure dephasing regime. We study the effect of various pulse sequences on the decoherence time for both weakly and strongly coupled fluctuators described by random telegraph noise (RTN). For a strongly coupled two-level system, the application of multiple pulses leads to a large enhancement of qubit coherence time. By theoretically comparing various dynamic decoupling schemes, we conclude that the Car-Purcell-Meiboom-Gill (CPMG) pulse sequence, well-known in NMR spectroscopy and recently discussed in the context of electron spin qubits in semiconductors [1], is the most optimal coherence-restoring scheme for the single fluctuator problem of relevance to superconducting qubits. We also find that for a large number of applied pulses the Gaussian approximation for the noise reproduces the exact results even in the strongly coupled regime.


This work is supported by the LPS-NSA-CMTC grant and by a fellowship from the Joint Quantum Institute (RL).

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H16 DBP DFD: Focus Session: Biochip Physics I Morial Convention Center 208

8:00AM H16.00001 Size Scaling of Protein Sensitivity on the BioCD, KEVIN O’BRIEN, MING ZHAO, XUEFANG WANG, DAVID NOLTE, Purdue University — We investigate size scaling of the surface-height sensitivity of spinning-disk interferometry (SDI) implemented on the in-line-quadrature BioCD as a function of laser focal radius. The in-line-quadrature BioCD consists of a silicon wafer with a 120 nm layer of silicon dioxide that creates a quadrature condition between the incident and reflected light. When a laser beam is focused on the BioCD, proteins printed on the silicon dioxide substrate create a phase shift leading to quadrature interference, which is detectable as an intensity shift. The purpose of this scaling experiment is to determine the practical and fundamental limits on the sensitivity of the BioCD, and how those limits change as a function of the size of the focal spot. We imaged a single 100 micron wide protein spot with focal spot sizes of 1, 5 and 10 microns and observe a square-root scaling as a function of the number of pixels per protein spot.

1NSF REU Program

8:12AM H16.00002 Detection Limits of Captured Protein on the BioCD, DAVID NOLTE, XUEFANG WANG, KEVIN O’BRIEN, MING ZHAO, Purdue University — The BioCD is an interferometric biosensor that detects protein captured by antibody arrays. The sensor readout is performed on a spinning disc using a common-path interferometric configuration that is stable and sensitive to sub-monolayer coverage of captured protein. Protein is detected using phase quadrature that converts phase to intensity modulation using local generation of signal and reference to lock the relative phase of the waves. The purpose for spinning is to move far from 1/f noise to achieve high surface mass sensitivity. Several different classes of the BioCD have been developed, differentiated by the means of generating the phase-locked reference. These include the microdiffraction (MD) class, the phase contrast (PC) class, the adaptive optical (AO) class and the in-line (IL) class of BioCD. Of these different quadrature classes, the in-line BioCD has the highest sensitivity with a detection sensitivity of 0.25 pg/mm. The minimum detectable mass is set by simple scaling relations. The metrology limit is set by surface roughness combined with repositioning offset between pre- and post-incubation scans. Optimal sensitivity is achieved by critical sampling of protein spots in radial arrays.

8:24AM H16.00003 Docetaxel-loaded Nanohorn-streptavidin-antibody for Anti-cancer Drug Delivery, JIANXUN XU, MASAKO YUDASAKA, MINFANG ZHANG, JST/SORST, NEC, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, SIMUO IJIMA, Meijo University, Nagoya 468-8502, Japan — Single wall carbon nanotube (SWNH) is a new kind of nano-carbon tubule having horn-like structure at its tip. The tube diameters are 2 to 5 nm, and about 2,000 SWNHs assemble to form a spherical aggregate. SWNH is an attractive candidate for drug delivery, especially promising to carry anticancer drug, many of which are not water soluble and highly toxic. We incorporated Docetaxel (Doc), an anticancer drug used for stomach cancer and others, into hydrogen peroxide treated SWNH (SWNHox). By using carboxylic groups on SWNHox, we attached amine-PEO3-biotin, and then streptavidin to biotin. The streptavidin moiety on SWNH makes it easy to attach some other biotinylated molecules, thus we introduced a cancer targeting ligand, anti-tumor associated glycopolypeptide, to the SWNH system. Due to the targeting effect of the antibody, the cells were effectively killed when they were incubated with the Doc SWNHox-streptavidin-antibody system.
8:36AM H16.00004 Detection limits and scalability of miniaturized antibody assays in real-world applications
BRIAN HAAB, Van Andel Institute — Antibody-based analytical assays have increasing importance in biological and biomedical applications. The ability to miniaturize the assays can lead to increased multiplexing and throughput, thus increasing information content while saving on the consumption of valuable samples and reagents. However, several challenges need to be addressed to enable the implementation of such technologies. This talk will address the factors affecting detection limits and scalability in real-world applications of antibody microarrays for the study of proteins in human blood serum.

9:12AM H16.00005 InAs quantum well μ-Hall sensors for magnetic biosensing
KHALED ALEDEALAT, S. HIRA, K. CHEN, Florida State Univ, G. MIHALOVIĆ, Materials Science Division, Argonne National Lab, P. XIONG, G. STROUSE, P.B. CHÄSE, S. VON MOLNAN, Florida State Univ, M. FIELD, C. SULLIVAN, Teltronic Scientific Company LLC — Magnetic sensing is potentially a sensitive and rapid technique for monitoring DNA-DNA and protein-DNA interactions. Here we present an effort on the noise characterization and selective biofunctionalization of InAs μ-Hall sensors for magnetic detection of DNA hybridization. Room-temperature noise measurements were performed in the frequency range from 20 Hz to 104 kHz. The noise equivalent magnetic moment resolution were estimated to be \( \sim 10^5 \mu_B/\sqrt{Hz} \) and \( \sim 10^4 \mu_B/\sqrt{Hz} \). The active region of the InAs μ-Hall device was covered with sputter-deposited SiO₂ and Au pads were patterned on top of some of the Hall crosses. Thiolated ssDNA were assembled on the Au pads and the rest of the device platform was passivated with PEG-silane. Biotinylated and fluorescently-tagged complementary ssDNA were labeled with commercial streptavidin-coated 350 nm superparamagnetic beads, which were found to assemble selectively onto the Au pads through DNA hybridization using laser scanning confocal microscopy. This work was supported by NIH NIGMS GM079592.

9:24AM H16.00006 Ligand-receptor binding kinetics in surface-plasmon resonance devices: A Monte Carlo simulation study
MATTHEW T. RAUM, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435, MANOJ GOPALAKRISHNAN, Harish-Chandra Research Institute, Allahabad 211019, India, KIM FORSTEN-WILLIAMS, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061-0435 — We use lattice Monte-Carlo simulations to probe the kinetics of ligand-receptor association and dissociation. Simulations were run under conditions approximating the geometric configuration of surface plasma resonance devices. These conditions include viscous flow of ligand over a surface of receptors which is achieved by using a spatially varying biased random walk. Our simulations allow for the occurrence of multiple rebinding events which result in long deviations from the standard mean-field rate equation approximation. Our simulations also allow us to test improved theoretical predictions for the binding dynamics and to determine their range of applicability.

3Research in part funded through the National Science Foundation, NSF DMR-0075725.

9:36AM H16.00007 Comparative study of different DNA chip preparation methods by means of Surface Plasmon Resonance
YANNICK SARTENAER, Laboratoire Lasers et Spectroscopies - FUNDP - University of Namur, 61 rue de Bruxelles, B-5000 Namur, Belgium, RUYJI HARA, HARUMA KAWAGUCHI, Laboratory of Polymer Chemistry - Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan, PAUL A. THIRY, Laboratoire Lasers et Spectroscopies FUNDP - University of Namur, 61 rue de Bruxelles, B-5000 Namur, Belgium — Recently, we demonstrated that SPR vibrational spectroscopy allows the detection of the specific recognition between the two molecules of a model ligand-protein biosensor. Moreover, we studied by this technique, the formation of thiolated single stranded DNA (ssDNA) monolayers immobilized on metallic substrates which are the basis for various biotechnology applications. Before going further into monitoring the hybridisation process in DNA based sensors, it is important to identify a preparation method providing good quality DNA chips with respect to the recognition process. Therefore, we performed investigations by Surface Plasmon Resonance (SPR). Practically, we used four different methods of chip preparation on gold surfaces and we measured the amount of deposited molecules when the sensor is exposed to a target DNA solution. By this way, we monitored for each case the sensitivity and the selectivity of the sensor by comparing the hybridisation of complementary and non complementary target ssDNA, respectively.

9:48AM H16.00008 Nanoscale Building Blocks for Bioensor Development
AMANDA J. HAES, Department of Chemistry, University of Iowa — The development of new technologies based on nano- and microscale phenomenon is important and significant for many reasons. One of the most prominent of these is biological sensors for the diagnosis of diseases, detection of environmental toxins, and drug discovery. Research in our group focuses on the microscopic and spectroscopic analysis of the optical properties of nanostuctures and their integration with microfluidic devices with applications in biological sciences. In this talk, we will show results for an optical sensor based on localized surface plasmon resonance spectroscopy. It will be demonstrated that this nanoparticle based sensor can be used to detect a variety of ligands, including a biomarker for Alzheimer’s disease.

10:24AM H16.00009 Predictive Model for Label-free Electrical Detection of Bio-molecules
PRADEEP NAIR, MUHAMMAD ALAM, School of Electrical and Computer Engineering, Purdue University — Biosensors based on MOSFETs, silicon nanowires, and carbon nanotube nanocomposites promise highly sensitive, dynamic, label-free, electrical detection of bio-molecules with potential applications in genomics and proteomics. Although tremendous improvements in sensitivity have been reported in electrical detection of bio-molecules, many aspects of experimentally observed sensor response (S) are unexplained within the theoretical frameworks of kinetic response or electrolyte screening. In this paper, we combine analytic solutions of Poisson-Boltzmann and reaction-diffusion equations to show that the electrostatic screening within an ionic environment limits the response of nanobiosensor such that \( S \sim c_1 \left( \ln(c_0) - \ln(c_f) + \ln(c_r) + \frac{pH}{D_F} \right) + c_2 \) where \( c_1 \) are geometry-dependent constants, \( c_0 \) is the concentration of target molecules, \( c_f \) the salt concentration, and \( D_F \) the diffusion dimension of sensor surface. Our analysis provides a coherent theoretical interpretation of wide variety of puzzling experimental data that have so far defied intuitive explanation and have important implications for the design and optimization of nanoscale biosensors.

10:48AM H16.00010 Hybrid CMOS/Microfluidic Dielectrophoresis and Magnetic Manipulator Chip
DAVID ISSADORE, Harvard School of Engineering and Applied Sciences (SEAS), THOMAS P. HUNT², Harvard Physics, KEITH A. BROWN, HARVEY SEAS, R.M. WESTERVELT, Harvard SEAS and Physics — We present hybrid CMOS/microfluidic chips that combine the biocompatibility of microfluidics with the programmability of CMOS integrated circuits (ICs). The chips use a two-dimensional array of RF-electrode pixels that use dielectrophoresis (DEP) to simultaneously and independently control the location of many objects, including biological cells and chemical droplets. We highlight our next generation of CMOS/microfluidic chips that combine a two-dimensional array of high voltage (50 V) RF pixels to produce large DEP forces, a microelectromagnetic matrix that can independently trap and move magnetic beads, and integrated temperature sensors. We describe the design, fabrication, and testing of the hybrid chips as well as ongoing work to interface and package the chips for robust biological and chemical experiments.

1Supported by the NCI MIT-Harvard CCNE [1U54CA11949] and by the DoD through the NDSEG Fellowship Program
2Currently at UC Berkeley Bioengineering
8:00 AM H17.00001 Linking enzyme conformational dynamics to catalytic function with single-molecule FRET, YAN-WEN TAN, JEFFREY A. HANSON, Dept of Chemistry, UC Berkeley, KARL DUDERSTADT, Biophysics Graduate Group, UC Berkeley, SUCHARITA BHATTACHARYYA, Dept of Chemistry, UC Berkeley, HAW YANG, Dept of Chemistry, Biophysics, UC Berkeley & Physical Biosciences Division, LBNL — Enzymes exhibit endurable conformational remodeling on a timescale comparable to their catalytic cycle. These conformational dynamics may be critical to the enzymes’ catalytic function. In adenylate kinase (AK) from E. coli, this involves a large-amplitude rearrangement of the enzyme’s lid domain. We use high-resolution single-molecule FRET developed in our laboratory to measure AK’s domain movements on its catalytic timescale. We utilize maximum entropy-based methods to remove photon-counting noise from raw data, so that the enzyme’s entire conformational distribution can be quantitatively recovered without a presumed model. Multiple sequence alignment suggests regularities between the conserved residues and their structural-functional roles. Armed with precise single-molecule FRET dynamics measurements and comprehensive bulk kinetic studies of the mechanism, we were able to quantitatively correlate AK’s stochastic lid dynamics with its deterministic catalytic rates. Implications on the structure-function conservation and protein engineering will be discussed.

8:12 AM H17.00002 Concentration-dependent Cu(II) binding to prion protein, MIROSLAV HODAK, NC State U, WENCHANG LU, JERRY BERNHOLC, NC State U and ORNL — The prion protein plays a causative role in several neurodegenerative diseases, including mad cow disease in cattle and Creutzfeldt-Jakob disease in humans. The normal function of the prion protein is unknown, but it has been linked to its ability to bind copper ions. Experimental evidence suggests that copper can be bound in three distinct modes depending on its concentration, but only one of those binding modes has been fully characterized experimentally. Using a newly developed hybrid DFT/DFT method [1], which combines Kohn-Sham DFT with orbital-free DFT, we have examined all the binding modes and obtained their detailed binding geometries and copper ion binding energies. Our results also provide explanation for experiments, which have found that when the copper concentration increases the copper binding mode changes, surprisingly, from a stronger to a weaker one. Overall, our results indicate that prion protein can function as a copper buffer. 1. Hodak, Lu, Bernholc, JCP, in press.

8:24 AM H17.00003 Solvable model of mechanical unfolding of proteins, OLEG VOROV, UNC at Charlotte, DENNIS LIVESAY, DONALD JACOBS, UNC at Charlotte — We present exact analytical results describing single-molecule experiments on mechanical unfolding of proteins within a realistic model [1]. The corresponding relation between the extension at a given temperature of the macromolecule and the applied force is derived [2]. The configuration partition function is calculated exactly for a distance constraint protein model that describes the beta-hairpin to coil transition. The resulting extension-force curve is derived, and the results agree with the data from the single-molecule pulling experiments.

8:36 AM H17.00004 Dynamical Transition in polypeptides, YUNFEN HE, ANDREA MARKELZ, University at Buffalo, SUNY, Buffalo, NY, USA — Two of the possible causes for the so called dynamical transition (the rapid increase in flexibility for biomolecules at ~ 200 K) are: thermally activated side chain diffusive motions with hydration dependent activation energies; or a glass transition in the biological water directly adjacent to the biomolecule. If the transition is strictly due to side chain activation, it should not depend on protein structure. Previously we demonstrated that the dynamical transition remains after tertiary structure was removed using THz time domain dielectric spectroscopy (0.2 -2.0 THz, 0.5-5ps). Here measurements on polyalanine as a function of chain length show that the dynamical transition does not occur for peptide length shorter than 5. However, the transition is observed for 5 mer and higher. Structural and simulation studies indicate that the 5 mer transiently occupies structured forms [1,2]. These results suggest that A) the dynamical transition is not due to thermally activated side chain motion and B) secondary structure is necessary for the dynamical transition. Secondary structure possibly induces sufficient ordering in the adjacent water to result in a fragile to strong glass transition resulting in increased protein flexibility [3].

8:48 AM H17.00005 Dynamically stable beta-sheets in Cu-initiated misfolding of α-synuclein, FRANCIS ROSE, MIROSLAV HODAK, JERRY BERNHOLC, NC State University — The human protein α-synuclein has been implicated as a central constituent in multiple neurodegenerative diseases. In Parkinson disease it is even thought to be the causative link. α-synuclein can be stimulated to aggregate into deleterious fibrillar structures by mutation, metal binding, and agitation. In particular, Cu$^{2+}$ has been found in high concentrations in neural tissues of Parkinson sufferers. We propose a scenario involving the metal ion Cu$^{2+}$ as the misfolding β-sheet initiator of fibrillogenesis. A model fragment of the metal-bound protein was investigated using DFT to obtain conformational details of the energetically favorable geometries. Feasible β-sheet structures incorporating the DFT geometries were explored using heuristic β-sheet guidelines and inverse kinematics. The resulting structures were tested for dynamic stability by simulating the fully solvated protein by classical MD constrained by the DFT geometries. Our results indicate that dynamically stable structures exist and that the metal binding is directly responsible for initiating misfolding.
9:00AM H17.00006 Dynamics of Lysozyme in Trehalose solutions, PAVAN GHATTY, The University of Akron, EDWARD C. UBERBACHER, Oak Ridge National Laboratory — Anhydrobiosis in Tardigrades and Nematodes has been a topic of constant interest and intrigue in the scientific community. An increase in the concentration of Trehalose has been attributed to the ability of some organisms to survive extreme conditions of temperature, pressure and pH. Although there exist many experimental studies attributing this effect to Trehalose, the molecular details governing the interaction between Trehalose and proteins remains unclear. We have conducted a 20ns study of Lysozyme in varying concentrations of Trehalose in water. Strong and weak hydrogen bonds and hydrophobic interactions between water, Trehalose and protein seem to dictate the interactions in the system. We have observed a hydrogen bonded network of Trehalose around the protein entrapping a layer of water between itself and protein. Lysozyme remains in a near-native conformation throughout the simulation giving hints on the ability of Trehalose in preserving the structure of proteins.

9:12AM H17.00007 Spectral and Hydration Dependence of Protein Dynamical Transition1, FERDINAND LIPPS, J. R. KNAB, JING YIN CHEN, YUNFEN HE, A. G. MARKElz, Physics, University at Buffalo, SUNY — The protein dynamical transition, a rapid increase in flexibility at ~200K, is hydration dependent suggesting that the transition may in fact be due to a transition in the surrounding water. Previously we have shown that the terahertz dielectric response is sensitive to the dynamical transition using terahertz time domain spectroscopy [1]. The broadband technique allows the determination of what motions are affected by the transition, that is whether long time scale motions such as side chain rotations, or faster vibrational motions. Here we examine both the frequency and hydration dependence of the protein dynamical transition for hydrated myoglobin powder for the 0.2 – 2.0 THz and 80-295 K ranges. The transition is observed in both the real and imaginary parts of the dielectric response. Our earlier measurements of solutions did not show a transition in the real part of the permittivity, likely due to bulk solvent dominating the index. There is a strong frequency dependence with hydration. While a slight transition is observed at frequencies higher than 1 THz which is nearly hydration independent, for frequencies below 1 THz the strength of the transition rapidly increases with hydration. [1] A. G. Markelz, J. R. Knab, Jing Yin Chen, Yunfen He, Chem. Phys. Lett. 442, 413 (2007).

9:24AM H17.00008 Vibrational Dynamics of Heme Model Compounds, ALEXANDER BARABANSCHIKOV, Northeastern University, TIMOTHY SAGE, Northeastern University, MINORU KUBO, PAUL CHAMPION, Northeastern University, JIYONG ZHAO, WOLFGANG STURHAHN, ERCAN ALP, Advanced Photon Source, Argonne, IL — Synchronous and laser-based measurements supported by DFT calculations identify vibrational modes of the iron atom in Fe(P)(Cl) and Fe(P)(Br). These compounds are large enough to capture many essential aspects of heme geometry and vibrations. On the other hand, porphine models are small enough to simplify the vibrational spectrum and enable accurate analysis using DFT methods. Nuclear resonance vibrational spectroscopy (NRVS) and femtosecond coherence spectroscopy (FCS) provide a rare opportunity to identify both dometing and Fe-hemide stretch components of the reaction coordinate with confidence. Correlation analysis between 4-coordinate and 5-coordinate compounds suggests significant mixing between Fe-ligand and heme modes. Comparison with the larger model Fe(III)(OEP)(Cl) reveals the effect of peripheral group substitutions.

9:36AM H17.00009 Ligand-Modulated Free Energy Landscapes of Glucose/Galactose Binding Protein1, TROY MESSINA, Centenary College of Louisiana — Glucose/galactose binding protein (GBP) functions as part of a larger system of proteins for molecular recognition and signaling in enteric bacteria. Here we report on the thermodynamics of conformational equilibrium distributions of GBP. From both time-resolved fluorescence experiments and computational umbrella sampling molecular dynamics analyses by the weighted histogram analysis method (WHAM). Three conformations appear at zero concentration of GBP and systematically transition to three conformations at high glucose concentration. Fluorescence anisotropy correlations, fluorescent lifetimes, thermodynamics, computational structure minimization and molecular dynamics, and previous work were used to identify the three components as open, closed, and twisted conformations of the protein. The existence of three states at all glucose concentrations indicates that the protein continuously fluctuates about its conformational state space via thermodynamically driven state transitions, and the glucose biases the populations by reorganizing the free energy profile. These results and their implications are discussed in terms specific and non-specific interactions GBP has with cytoplasmic membrane proteins.

9:48AM H17.00010 Ligand Binding Kinetics in Myoglobin and Solvent Relaxation at High Pressure, ALFONS SCHulte, University of Central Florida, SILKI ARORA, SANGHOON PARK — Pressure is increasingly used as a variable to examine protein structure-function relationships, since it is crucial for chemical equilibria, reaction rates, and protein conformational states. We investigate pressure effects for the prototype reaction of ligand binding to myoglobin over a wide dynamic range in time and temperature. The distribution of rebinding rates is evaluated from terahertz time domain spectroscopy (THz-TDS) measurements of Fe(III)(OEP)(Cl) and Fe(III)(OEP)(Br) myoglobin for the 0.1 – 1.0 GPa pressure range and temperature (180 – 300 K) in aqueous and 75 % glycerol/buffer solutions. The data demonstrate that pressure significantly affects the amplitudes (not just the rates) of the component processes. The amplitude of the geminate process increases with pressure corresponding to a smaller escape fraction of ligands into the solvent and a smaller inner barrier. Solvent relaxation rates at variable pressure are determined independently from specific heat spectroscopy. We discuss the role of solvent dynamics, hydration shell, and internal protein cavities in the binding reaction.

10:00AM H17.00011 Magnetic Hyperfine Interactions in Heme Unit of Metmyoglobin, N.B. MAHARJAN, Tribhuvan University, Nepal, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Upsala University, Sweden, R.H. PINK, SUNY Albany, LEE CHOW, A. SCHULTE, H.P. SAHA, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — The 14N and 57Fe hyperfine interactions in the heme unit of metmyoglobin are available experimentally by electron-nuclear double resonance (ENDOR) and Mossbauer spectroscope techniques. We have carried out electron structure investigation on the heme system including the H2O and proximal imidazole ligands by the first-principles Hartree-Fock procedure and studied the magnetic hyperfine and nuclear quadrupole coupling constants for the 57Fe nucleus and all the six 14N nuclei on the four pyrrole and imidazole ligands as well as the 17O nucleus on the H2O ligand. Comparison will be made with available experimental data [1, 2] and earlier theoretical investigations [3] by the approximate self-consistent charge Extended Hückel procedure. Results will also be presented for the optical frequencies and intensities of transitions between ligand-like and iron d-like states and the Fe-N, vibrational frequency [1]. G. Lang, Q. Rev. Biophys. 3 (1970) [2] C.P. Scholes, R.A. Isaacson and G Feher, Biochim. Biophys. Acta 263:448(1972) [3] S.K. Mun, Jane C. Chang and T.P. Das J. Am. Chem. Soc. 101, 5562(1979).

10:12AM H17.00012 Hartree-Fock Investigation of Electronic Structure and Associated Properties of Heme Unit in Deoxyhemoglobin, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, K. RAMANI LATA, SUNY Albany, R.H. SCHEICHER, Upsala University, Sweden, R.H. PINK, SUNY Albany, A. SCHULTE, LEE CHOW, H.P. SAHA, UCF Orlando, K. NAGAMINE, UC Riverside, T.P. DAS, SUNY Albany, UCF Orlando — Using the Hartree-Fock-Roothaan procedure and the most recent version of the Gaussian set of programs we have studied the electronic structure of the heme unit including the imidazole ligand of iron from the proximal histidine using x-ray data for the positions of all the atoms except the hydrogen. The positions of the latter have been obtained through energy optimization. The results obtained from the calculated electronic structure for the magnetic and electronic hyperfine interactions of the 57Fe and 14N nuclei will be discussed. Comparison will be made with available experimental data and earlier theoretical investigations [1]. Results will also be presented for the proximal Fe-N, vibrational frequency and the frequencies and intensities of optical transitions between ligand like states and d-like states of Fe [1]. K Ramani Lata PhD Thesis SUNY Albany (1993) (Unpublished).


Tuesday, March 11, 2008 8:00 AM - 11:00 AM — Session H18 DPOLY: Block Copolymers in Solution and Blends Morial Convention Center 210

8:00 AM H18.00001 Polymer Physics Prize Break

8:36 AM H18.00002 Competitive Adsorption, Exchange and Binding of Polymers and Proteins at the Oil/Water Interface. Daniel Carvajal, Kenneth Shull, Igal Szleifer, Northwestern University — Drop Shape Analysis (DSA) of pendant drops was used to study competitive adsorption, exchange kinetics and binding of macromolecules at the oil/water interface. Amphiphilic diblock and triblock copolymers were dissolved in the oil drop phase, while proteins were added to the water phase. By using DSA to monitor the interfacial tension of the system, we were able to gather data on how the polymers and proteins are behaving and interacting at the oil/water interface. Some polymer systems were found to fully inhibit both specific and non-specific adsorption of proteins to the interface. Adding biological receptors to these polymers allowed us to study the specific binding of proteins to polymers located at the interface. In other systems, proteins were able to penetrate the amphiphilic block copolymer layer and reach the interface. The dynamics of exchange and competitive adsorption in these polymer/protein systems were also studied.

8:48 AM H18.00003 Interfacial Properties of Semifluorinated Alkane Diblock Copolymers. Flint Pierce, Dvora PERAHA, Department of Chemistry Clemson University. MESPIN TSIGE, Department of Physics Southern Illinois University. Oleg Borodin, Department of Materials Science and Engineering and Department of Chemical and Fuels Engineering University of Utah. Gary Grest, Sandia National Laboratory — The surface interaction of semifluorinated alkane diblock copolymers with water and normal alkanes are studied using explicit atomistic molecular dynamic (MD) simulations. At the diblock/air interface, the surface is dominated by fluorinated alkane chains, with a low surface tension, and these groups reside at the interface for longer periods of time than the hydrogenated groups. Flouroalcohols even a single end group on an otherwise hydrogenated chain results in low surface tensions, close to that of perfluoroalkanes and far from normal alkanes. For the interface with water, results for the rate of water uptake by alkanes, perfluoroalkanes, and SFAs will be presented. Additionally, we report the interfacial surface tensions and equilibrium density profiles for these samples, focusing on the prevalence of fluorinated and hydrogenated segments at each interface. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04 - 94AL85000.

9:00 AM H18.00004 Amphiphilic copolymer assemblies formed by interfacial instabilities of oil-in-water emulsions. Jintao Zhu, Ryan C. Hayward, Department of Polymer Science and Engineering, University of Massachusetts at Amherst — Self-assembly of amphiphiles into discrete nano-objects is of fundamental interest and is important for applications including encapsulation and drug delivery. We will discuss a new method by which amphiphilic block copolymers can be controllably assembled into hierarchically-structured microparticles and various micellar morphologies. We first form oil-in-water emulsion droplets, where the dispersed phase consists of a volatile organic solvent containing a dilute concentration of amphiphilic polystyrene-block-poly(ethylene oxide) diblock copolymer. Upon extraction of the organic solvent, the droplets undergo interfacial instabilities which lead to formation of microparticles with budding vesicle, foam-like, or dendritic structures, or micelles with spherical, cylindrical, or more complicated morphologies. We will discuss the structure of these assemblies can be tuned, and the difficulties that they present for encapsulation of hydrophobic species.

9:12 AM H18.00005 Helical cylinders or multicompartment cylinders through the solution assembly of charged block copolymers with multivalent organic counterions. Darrin Pochan, Sheng Zhong, University of Delaware. Honggang Cui, Northwestern University. Zhiyuan Chen, Rhodia. Karen Woolley, Washington U. St. Louis — By manipulating the interaction of charged block copolymer hydrophilic corona blocks with multivalent organic counterions, and controlling the kinetics of block copolymer solution self-assembly, desired micelle geometries can be formed. Specifically, polyacrylic acid-b-poly(methylacrylate-b-polyethylene oxide) amphiphilic triblock copolymers were studied in water/THF solvent mixtures with organic multianions as counterions. By manipulating block copolymer and solvent composition, different micelle geometries were formed. However, by altering the chemical structure and/or concentration of the multianion counterions, as well as the kinetic pathway through which the molecules are assembled, complex nanostructures were formed. An example of nanostructure from kinetic control includes spherical micelles that can be controllably assembled into 1-d multicompartment cylinders. Examples of nanostructure from control of the type and amount of multivalent organic counterion added are helical cylinder superstructures many micrometers in length. The system has been investigated by means of cryogenic transmission electron microscopy (cryo-TEM) and small angle neutron scattering (SANS).}

9:24 AM H18.00006 Spotted Polymersomes and Striped Worms - a theoretical analysis of lateral segregation of diblock copolymers. Wouter G. Ellenbroek, Department of Physics and Astronomy, University of Pennsylvania. David A. Christian, Aiwei Tian, Chemical & Biomolecular Engineering and the Laboratory for Research on the Structure of Matter, University of Pennsylvania. Andrea J. Liu, Department of Physics and Astronomy, University of Pennsylvania. Tobias Baumgart, Dennis E. Discher, Chemical & Biomolecular Engineering and the Laboratory for Research on the Structure of Matter, University of Pennsylvania — Lipids and amphiphilic block copolymers are both known to assemble into vesicle and worm-like micelle morphologies, but only mixtures of lipids in vesicles have been directly seen to phase separate into meso-scale lateral domains. Here we show direct visualization of meso-scale spots in tough polymersomes and microphase separated diblock copolymers, which result from strong lateral segregation of polyamionic and neutral diblock copolymers. We present a model for understanding the crucial role of calcium ions on segregation behavior, which incorporates counterion condensation and “crosslinking” (ion bridging). We find a tendency towards segregation near the isoelectric point as a result of competition among counterion entropy, repulsion due to the net charge, and attraction due to crosslinking. These results portend new classes of robust membranes and cylinders that exhibit lateral patterns at the meso-scale.
9:36AM H18.00007 Pathways of Spontaneous Vesicle Formation of ABA Amphiphilic Molecules in Selective Solvent. — WEI JIANG, HONGBO DU, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We study the pathways of spontaneous vesicle formation of the ABA amphiphilic molecules in selective solvent by Monte Carlo simulation. Simulation results reveal that the pathway for the spontaneous vesicle formation of the amphiphilic molecules in selective solvent depends strongly on the annealing speed. We can not use one pathway model to describe the vesicle formation even though for the same system and condition. Hydrophobic molecules diffusing in spherical micelles and oblate membrane closing may coexist for the vesicle formation.

9:48AM H18.00008 Effects of depletion interactions on block copolymer micelles. — SAYEED ABBAS, TIMOTHY P. LODGE, Department of Chemical Engineering and Materials Science, University of Minnesota — Block copolymer micelles exhibit two levels of hierarchical self-assembly: the process of micellization itself, and the ordering of these micelles onto a lattice. By a combination of small angle x-ray scattering and neutron scattering, we show that both levels of self-assembly are affected when non-adsorbing homopolymer is added to the solutions. The phenomena are analogous to depletion interactions in colloid/polymer mixtures. We have chosen poly(styrene-b-isoprene) micelles dissolved in diethyl phthalate as the model system. To these solutions polystyrene homopolymer was added. The effects strongly depend on the molecular weight and concentration of the added homopolymer. We find an induced attraction between micelles at moderate micelle concentrations, and a preference for fcc over bcc lattices in more concentrated solutions.

10:00AM H18.00009 Influence of Electric Fields on the Phase Behavior of Concentrated Block Copolymer Solutions. — KRISTIN SCHMIDT, HEIKO SCHOBERTH, ALEXANDER BOKER, University Bayreuth — We investigate the influence of the electric field on the phase behavior of diblock copolymer concentrated solutions using synchrotron SAXS. We find a significant dependence of the characteristic domain spacing on the electric field strength. For lamellae aligned parallel to the electric field direction we observe that the lamellar spacing decreases with increasing field strength, while for perpendicularly oriented lamellae the domain spacing increases. We also find that the electric field can induce an order-order transition if the block copolymer has a composition close to the predicted phase boundary. Due to the lower free energy of aligned anisotropic microdomains structures parallel to the electric field, we can induce a transition from the metastable hexagonally perforated lamellar phase to the lamellar phase without perforations by applying strong electric fields. Similarly an isotropic cubic gyroid phase, which is stable in the absence of, but cannot be aligned by, the field, transforms to aligned cylinders when a strong electric field is applied.

10:12AM H18.00010 Well Ordered Melts from Low Molar Mass Pluronic Copolymers Blended with Poly (acrylic acid): Effect of Homopolymer Molar Mass. — VIKRAM DAGA, University of Massachusetts - Amherst, VIJAY TIRUMALA, Polymers Division, National Institute of Standards and Technology, ALVIN ROMANG, University of Massachusetts - Amherst, ERIC LIN, Polymers Division, National Institute of Standards and Technology, JAMES WATKINS, University of Massachusetts - Amherst — The use of short chain block copolymer melts as nanostructured templates is often limited by their low segregation strength. We have recently shown that block copolymer melts with a molar mass less than 15 kg/mol undergo disorder-to-order transition without a significant increase in interdomain spacing when blended with a selectively associating homopolymer, due to an apparent increase in effective \(\chi\). Here, we study the effect of homopolymer molar mass on the segregation of a disordered poly (oxyethylene-oxypropylene-oxyethylene) copolymer melt that forms lamellar microstructure in the ordered phase. Based on small-angle scattering measurements, we find that the melts remain ordered over a broad range of homopolymer chain lengths, ranging up to ten times that of the copolymer. This approach has many implications for the use of commodity block copolymer surfactants as inexpensive nanostructured templates for commercial applications.

10:24AM H18.00011 Novel Characterization of Critical Micelle Concentrations of Block Copolymers and Gradient Copolymers in Homopolymer. — ROBERT SANDOVAL, DANIEL WILLIAMS, CHRISTOPHER WONG, JUNGKI KIM, JOHN TORKELSON, Northwestern University — Here we demonstrate a new method based on the intrinsic fluorescence of styrene-containing block copolymers and gradient copolymers to determine the critical micelle concentrations (cmc) of copolymers present at low levels in homopolymer. The method relies on the fact that the when styrene/methyl methacrylate (S/MMA) block copolymers and gradient copolymers are well dispersed in a glassy homopolymer such as poly(methyl methacrylate) (PMMA), only monomer fluorescence and no excimer fluorescence is observed from the copolymers. When micellization occurs, then excimer fluorescence is present. With this simple method, we have found that gradient copolymers yield much lower cmc values (about an order of magnitude smaller) than comparable block copolymers of similar molecular weight and overall composition. We are extending these studies to consider the effects of block copolymer molecular weight and composition as well as homopolymer molecular weight on the cmc values. While these parameters have received heavy consideration from a theoretical standpoint, little experimental work has focused on these issues.

10:36AM H18.00012 The influence of macromolecular architecture on the micellization in block copolymer/homopolymer blends. — E. PAVLPOULOUI, K. CHRISSOPOULOUI, S.H. ANASTASIADIS, G. PORTALE, W. BRAS, ESF-DUBBLE, Grenoble, France, H. IATROU, S. PISPAS, N. HADJICHRISTIDIS, Univ. of Athens, Greece — We investigate the micellar formation and micelle characteristics of block copolymers of varying architecture within homopolymer matrices. A series of symmetric (polyisoprene) \((I_nS_n)\), (polystyrene) \((S_nI_n)\), and (methyl methacrylate) \((I_nS_n)\) mictom star block copolymers, with \(n\) identical pairs of arms, and a series of \((\text{polysoprene})_2\) (polystyrene), \(I_2S\), graft copolymers with constant total MW and varying composition, \(f_{PS}\), are added to a low MW PI homopolymer matrix and the blends are investigated by small-angle X-ray and light scattering as a function of copolymer concentration and \(f_{PS}\). The functionality of the junction point of the copolymer does not influence the characteristics of the \(I_nS_n\) micelles, while \(f_{PS}\) controls the behavior of the \(I_2S\) grafts. A simple thermodynamic model is developed that describes theoretically the micellization of \(A_B\) copolymers within B homopolymers and its predictions agree very well with the experimental data both qualitatively and quantitatively. Sponsored by NATO’s Scientific Affairs Division, by the Greek GSRT and by the EU.

10:48AM H18.00013 Phase Behavior and Dimensional Scaling of Symmetric Block Copolymer-Homopolymers Ternary Blends in Thin Films. — GUILIANG LIU, MARK STOYKOVICH, SHENXIANG JI, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, 1415 Engineering Drive, Madison, WI, 53706 — We have studied the phase behavior and dimensional scaling of symmetric ternary blends of PS-PMMA block copolymers and the respective PS and PMMA homopolymers in thin films. Below the order disorder transition (ODT) temperature, the symmetric ternary blends form lamellae, microemulsion and macrophase separated phases as a function of \(\chi N\), \(\alpha\) (a ratio of degree of polymerization of homopolymers to that of the block copolymer), and \(\phi_H\) (volume fraction of homopolymers). The phase transition compositions from lamellae to microemulsion and from microemulsion to macrophase separation depend weakly on \(\chi N\) and \(\alpha\) in the range of \(12.7 \leq \chi N \leq 37.6\) and \(0.20 \leq \alpha \leq 0.99\). The dimensions of swollen lamellae and microemulsion \((L_0)\) can be determined as a function of \(\phi_H\) and \(\alpha\), explicitly, \(L_0 = L_{0h}/(1-\phi_H)^{b}\), where \(L_{0h}\) is the natural bulk period of pure block copolymer, and \(b\) is a parameter depending strongly on \(\alpha\).
8:00AM H19.00001 Competition between intermolecular and substrate interactions in a multi-component lattice gas model. QIANG LIU, University of Maryland at College Park, JOHN WEEKS, University of Maryland, E.D.WILLIAMS'S GROUP, J.REUPT-ROBEY'S GROUP TEAM — Recent experiments have shown that acidine-9-carboxylic acid (ACA) molecules form a dense phase consisting of chain-like structures on Ag(111) with alternating orientations along the chain direction that permit the formation of strong hydrogen bonds. Despite the anisotropy in intermolecular interactions that leads to chain formation, molecular boundaries along and normal to the chain direction have very similar thermodynamic properties and fluctuations. We introduce a multicomponent lattice gas model where molecules with different orientations are treated as different species with different intermolecular interactions as well as different interactions with the substrate. This a generalization of the familiar Blume-Emery-Griffiths model of a binary lattice gas but in a region of parameter space not usually explored. We argue that the novel domain shapes, boundary fluctuations and phase densities seen in experiment arise from a competition between favorable anisotropic pair interactions in the chain phase and less favorable substrate interactions due to the different orientations. Detailed results of Monte Carlo simulations of this model and analytic work using mean field and pair approximation theories will be presented.

Work supported by the UMC NSF-MRSEC grant DMR 05-20471

8:12AM H19.00002 Van der Waals interactions at the molecule-metal interface: PTCDA on Ag(111). LORENZ ROMANER, DIMITRI NABOK, PETER PUSCHNIG, Department of Materials Physics, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria — EGBERT ZOJER, Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria, CLAUDIA AMBROSH-DRAXL, Department of Materials Physics, University of Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria — A detailed understanding of the processes governing the adsorption of molecules on metallic surfaces is of major interest for the field of molecular electronics. In this context, the molecule 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) has been extensively studied on a variety of metallic surfaces and has so gained fundamental, academic importance. The theoretical description of the adsorption is, however, still controversial as standard density functional theory (DFT) does not include van der Waals interactions, which, for PTCDA and many other molecules, yields the dominant binding contribution. We present DFT calculations of PTCDA adsorbed on Ag(111) where a recently developed exchange-correlation functional was adopted to include van der Waals interactions. Adsorption energy and distances, molecular distortions, charge rearrangements and orbital occupancies are discussed in detail.

8:24AM H19.00003 Tilt Angle Determination in Thin Films with Anisotropic Molecules. THOMAS GREDIG, Dept of Physics, California State Univ, Long Beach, CA 90840, GE LIU, IVAN K. SCHULLER, Dept of Physics, University of California, San Diego, La Jolla, CA 92039 — Many electronic properties of organic semiconductors depend critically on their physical and chemical arrangement of atoms. Here, a method is described to extract information about the molecular tilt angle and to determine the center electron density of anisotropic molecular thin films by means of specular x-ray diffraction. Thin films of phthalocyanine (Pc), an anisotropic molecule with a metal ion in the center, have been deposited in an organic molecular beam deposition system and studied with high-resolution x-ray diffraction. In particular, two isomorphous molecules, H2-Pc and Cu-Pc, are compared experimentally and then studied with numerical simulations. The results show that the intensity distribution of the diffraction peaks belonging to the same series of lattice planes provides important structural information such as the molecular tilt angle or the center electron density of the anisotropic molecule.

This work is supported by AFOSR-MURI grant No. F.49620-02-1-0288.

8:36AM H19.00004 The role of defects and phonons in O2 adsorption on Cu(100). MATTI ALATALO, ANTTI PIUSTO, Lappeenranta University of Technology — We present the results of an extensive ab initio study for O2 adsorption on the Cu(100) surface. The calculated potential energy surfaces and first principles molecular dynamics trajectories reveal that on the clean surface without defects the dissociation probability is low at small translational energies of the incoming molecule whereas at higher energies the molecules dissociate directly without a barrier. Of the different defects, steps turn out to be less reactive than expected and adatoms rather lower than enhance the reactivity. In contrast, vacancies act as dissociative centers, which locally enhance the reactivity. This result is in agreement with the molecular beam surface scattering experiments which show an increase at the oxygen sticking probability at low energies. We also discuss the role of phonons in O2 dissociation, showing that the open space involved at certain phonon modes lowers the dissociation barrier, an effect analogous to the vacancy induced dissociation. Our results clearly demonstrate the importance of including both defects and surface dynamics in a realistic description of the adsorption process.

8:48AM H19.00005 Vibrational spectroscopy and ab initio dynamics of the O-induced added-row reconstructed Cu(110) surface. TALAT S. RAHMAN, M. ALCANTARA ORTIZOZA, University of Central Florida, R. HEID, K.P. BOHNNEN, Forschungszentrum Karlsruhe, K. BRUEGEMANN, H. IBACH, Forschungszentrum Juelich — It is known that O2 molecules dissociatively adsorb on Cu(110) and, upon subsequent annealing, Cu and O atoms catenate along the [100] direction arranging themselves in a striped periodic super-grating, depending on O coverage and annealing temperature. It has been proposed that stress along the [110] direction in the regions that locally hold a (2x1)O added-row on Cu(110) and, upon subsequent annealing, Cu and O atoms catenate along the [100] direction arranging themselves in a striped periodic super-grating, depending on O coverage and annealing temperature. We present DFT calculations of PTCDA adsorbed on Ag(111) where a recently developed exchange-correlation functional was adopted to include van der Waals interactions. Adsorption energy and distances, molecular distortions, charge rearrangements and orbital occupancies are discussed in detail.

Work supported in part by NSF under grant CHE-0548632.

9:00AM H19.00006 Insights from surface stress calculations on the structure of c(2×2)-N overlayer on Cu(001). SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We present results of calculated changes in surface stress for N overlayers on Cu(001), in an effort to discriminate between several proposed structural models. Our calculations of the surface geometry and electronic structure are based on the density functional theory in the generalized gradient approximation and the pseudopotential method. We find that a c(2×2) N overlayer causes a large change in the surface stress (≈ 5 N/m) on Cu(001) turning it from tensile to compressive. We also perform calculations for several stress relief models to find that the so-called “rumpling” and “clock reconstruction” models fail to relieve the N induced stress. On the other hand, formation of strips of clean Cu(001) areas, aligned along the [100] direction, and trench-like steps of Cu atoms, along the [110] direction on Cu(001), relieve the induced stress most effectively, in agreement with predictions from experiments. We consider the implications of these results on surface phonon dispersion curves for unreconstructed c(2×2)-N/Cu(001), which are in good agreement with experiment.

Work supported in part by NSF under grant CHE-0548632.
9:12AM H19.00007 First principles calculations of the vibrational dynamics of c(2x2)-CO on Ag(001).1 M. ALCANTARA ORTIGOZA, T.S. RAHMAN, University of Central Florida, R. HEID, K.P. BOHNEN, Forschungszentrum Karlsruhe, Germany — The reaction pathway of CO oxidation on Ag surfaces is still a subject of debate because of the complicated chemistry of O and the possibility that contaminants stabilize CO. Indeed, at ~150 K, the dissociative O₂ adsorption is scarcely triggered while the CO adsorption on clean Ag(001) is hardly stable. The nature of the CO adsorption is thus by itself a matter of discussion and the characteristic energy losses for exciting the phonon modes introduced by the adsorbed species have an uncertain assignment. We present an ab initio study of the structure and phonon dispersion of a c(2x2), atop, CO overlay on Ag(001). Comparison with a similar study of c(2x2) CO on Cu(001) indicates that CO chemisorbs on Ag(001) despite the low binding energy. The frequency of the C-O stretch mode at the Γ-point is in excellent agreement with HREELS measurements and is reduced on Ag(001) almost as much as on Cu(001). The weak Ag-CO bond is reflected in the low frequency of the rest of the CO modes. Yet, in the Ag-CO stretch, the Ag surface atoms are strongly coupled, as in the case of CO on Cu(001). Likewise, the CO frustrated translation mode couples to the substrate in the vicinity of the Γ-point but, unlike that on Cu(001), the CO frustrated rotation mode on Ag(001) couples to the substrate inside the surface Brillouin zone.

1Work supported in part by NSF under grant CHE-0548632.

9:24AM H19.00008 Oxygen-Induced Reconstructions on the β-Si₃N₄ (10̂10) Surfaces , WERONIKA WALKOsz, JUAN CARLOS IDRÓBO, SERDAR OGUT1. University of Illinois at Chicago — Motivated by recent electron microscopy studies at the Si₃N₄/rare-earth oxide (REO) interfaces, we present first principles calculations for the preferred bonding sites and configurations of oxygen on various terminations of the β-Si₃N₄ (10̂10) surface as a function of coverage and surface stoichiometry. We predict that oxygen induces various surface reconstructions, and it has a strong tendency to replace N on the surface. The structural stability of most low-energy surface structures is driven by the tendency of Si to saturate its dangling bonds and of oxygen to bridge two Si atoms similar to the bonding in SiO₂. The present ab initio results resolve the discrepancy between the experimental observations at the Si₃N₄/REO interfaces and previous theoretical studies for bare surfaces regarding the lowest energy surface termination.

1Supported by NSF Grant No. DMR-0604964

9:36AM H19.00009 Insight into water molecules bonding on 4d metal surfaces , JAVIER CARRASCO, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany, ANGELOs MICHAELIDES, MATTHIAS SCHEFfLER — Water-metal interactions are of capital importance to a wide variety of phenomena in materials science, catalysis, corrosion, electrochemistry, etc. Here we address the nature of the bond between water molecules and metal surfaces through a careful systematic study. Specifically, the bonding of isolated water molecules to a series of close-packed transition metal surfaces - Ru(0001), Rh(111), Pd(111) and Ag(111) - has been examined in detail with density functional theory (DFT). Aiming to understand the origin behind energetic and structural trends along the 4d series we employ a range of analysis tools, such as decomposition of the density of states, electron density differences, electronic reactivity function and inspection of individual Kohn-Sham orbitals. The results obtained allow us to rationalize the bonding between water and transition metal surfaces as a balance of covalent and electrostatic interactions. A frontier orbital scheme based on so-called two-center four-electron interactions between molecular orbitals of water and d band states of the surface proves incisive in understanding these systems.

9:48AM H19.00010 Water uptake on thin film MgO using ambient pressure XPS, JOHN T. NEWBERG, DAVID E. STARR, ERIN MYSAK, Lawrence Berkeley National Laboratory, SÜSUMU YAMAMOTO, ANDERS NILSSON, Stanford Synchrotron Radiation Laboratory. HENDRIK BLUHM, Lawrence Berkeley National Laboratory, LAWRENCE BERKELEY NATIONAL LABORATORY TEAM, STANFORD SYNCHROTRON RADIATION LABORATORY TEAM — Understanding the molecular level interactions of water with metal oxide surfaces is important in both industrial processing and environmental chemistry. MgO(100) is one of the most widely studied metal oxide surfaces due to its simple rock salt cubic structure. However, whether water adsorbs dissociatively (hydroxylation) or molecularly (thin film wetting) remains unanswered. We have characterized the uptake of water on 7ML MgO(100) on Ag(100) at RT using ambient pressure XPS. Surface compositions were measured in-situ under water vapor pressures ranging up to 1 Torr. Our results indicate that initial hydroxylation occurs at low pressures mostly at Mg(2+) sites up to about 0.1 mTorr. At higher coverages both hydroxylation and thin film wetting continues through 1 Torr. We will also discuss results from: 1. water uptake under higher/lower effective vapor pressures, 2. additional MgO(100) film thickness, and 3. water uptake on MgO(111)/Ag(111) surfaces.

10:00AM H19.00011 Surface-induced solid-phase transitions in ultra-thin water films at T > 0 °C, ANIMEsh CHAKRABORTY, ANDREW GELLMAN, LAYTON BAKER, ESTEBAnH BROITMAN, carnegie Mellon University — We report here the measurements of both the adsorption isotherms and the dissipation in ultra-thin films of water adsorbed on the surfaces of SiO₂. The measurements were made in a small high vacuum chamber in which we have mounted a QCM. The chamber was evacuated to ~10⁻⁸ Torr (the vapor pressure of water at room temperature is ~22 Torr). In addition the temperature of the apparatus can be varied in the range 10 – 60 °C. This is sufficient to measure the adsorption isotherm and to probe the phase of adsorbed water films over the range of conditions. Recently published work studying the adsorption of water on the SiO₂ layer formed on Si single crystals has suggested that the phase of the water at temperatures well above 0 °C is actually that of a solid, ice-like structure rather than liquid water [1]. That work is based on the comparison of the vibrational spectrum of thin water films with those of liquid water and ice. In our study we are using the QCM to investigate the possibility of formation of Ice-like structures. However, whether water adsorbs dissociatively (hydroxylation) or molecularly (thin film wetting) remains unanswered. We have characterized the uptake of water on 7ML MgO(100) on Ag(100) at RT using ambient pressure XPS. Surface compositions were measured in-situ under water vapor pressures ranging up to 1 Torr. Our results indicate that initial hydroxylation occurs at low pressures mostly at Mg(2+) sites up to about 0.1 mTorr. At higher coverages both hydroxylation and thin film wetting continues through 1 Torr. We will also discuss results from: 1. water uptake under higher/lower effective vapor pressures, 2. additional MgO(100) film thickness, and 3. water uptake on MgO(111)/Ag(111) surfaces.


10:12AM H19.00012 Relaxation of the (111) Surface of δ-Pu and Effects of Atomic Adsorption: An Ab Initio Study1 RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — The full-potential all-electron linearized augmented plane wave plus local orbitals (FP-LAPW+lo) method has been employed to study the relaxation of the δ-Pu (111) surface and the consequent effects for atomic adsorption of C, N and O atoms on this surface. The surface was modeled by a 5-layer slab with a (2x2) surface unit cell. Upon relaxation of the surface, the interlayer separation between the surface and the subsurface layers expanded by 7.1% with respect to the bulk interlayer separation while the separation between the subsurface and central layers expanded by 0.4%. The hollow fcc adsorption site was found to be the most stable site for C and N with chemisorption energies of 6.420 eV and 6.549 eV respectively, while the hollow fcc adsorption site was found to be the most stable site for O with a chemisorption energy of 7.858 eV. The adsorbate-induced changes in the surface properties, namely the Pu magnetic moments, work function, and electronic structure will be discussed.

1This work is supported by the U. S. Department of Energy and the Welch Foundation.
by thermal diffusion. Sites formed by single HV or pairs of adjoining HVs were found to be unreactive toward H₂. Thanks to LT-STM atomic observations, we show that this new description of H₂ dissociative adsorption onto transition metal surfaces is not an exotic particular catalytic case relevant only to Pd(111) and close-packed faces of fcc metals, but that it also applies to close-packed faces of hcp metals such as Ru(001) [1, 2]. Close to saturation of 1 ML, HVs were observed either as single entities or forming transient aggregations. Vacancies diffuse and aggregate to form active sites for the dissociative adsorption of H₂. We have found that H₂ dissociation takes place only on Ru sites where the metal atom is not bonded to any H atom [3]. Such active sites are formed when at least 3 HVs aggregate by thermal diffusion. Sites formed by single HV or pairs of adjoining HVs were found to be unreactive toward H₂. [1] T. Mitsui, et al., Nature 422 705 (2003) [2] M. Tatarkhanov, et al., Surf. Sci., in Press (2007) [3] F. Rose, et al., J. Phys. Chem. C, Accepted (2007)

3 This research was supported by NSF grant CHE040001 and the computations were performed in part on the Cray XT3 (Big Ben) at the Pittsburgh Supercomputing Center.

Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H20 DMP: Focus Session: Assembly of Nanowires and Related Structures Morial Convention Center 212

8:00AM H20.00001 Formation and Properties of CdS-Ag₃S Nanorod Superlattices¹. DENIS DEMCHENKO, RICHARD ROBINSON, BRYCE SADTLER, LIN-WANG WANG, A. PAUL ALIVISATOS, Lawrence Berkeley National Laboratory, CAN ERDONMEZ, University of California, Berkeley — The mechanism of formation of recently fabricated ordered CdS-Ag₃S nanorod superlattices is explained and their elastic and electronic properties are predicted theoretically. We show that diffusion-limited growth of Ag₃S islands in CdS nanorods partially contributes to the observed ordering, but cannot account for the full extent of the ordering alone. The valence force field (VFF) model results for the nanostructure show significant repulsion between Ag₃S segments due to strain created by the lattice mismatch between the two materials. This suggests that the interplay between the chemical interface energy and strain drives the spontaneous pattern formation. A first principles calculation of the energy levels in the superlattice shows a nested band alignment. The nanorod superlattice therefore corresponds electronically to a sequence of quantum wells of Ag₃S separated by barriers of CdS. The minibands formed in such superlattices make them desirable for applications in the solar cells. 1. R. D. Robinson, B. Sadtler, D. O. Demchenko, K. C. Erdonmez, L.-W. Wang, and A. P. Alivisatos, Science 317, 355 (2007).

1Supported by U.S. DOE, No. DE-AC02-05CH11231 and NERSC.

8:12AM H20.00002 Transport studies on ultrathin silicide nanowires. VOLTAIA IANCU, CHANGGAN ZENG, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN, 37996, STEPHEN JESSE, ARTHUR BADDORF, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, HANNO WEITERING, Department of Physics and Astronomy, University of Tennessee, Knoxville, TN, 37996 — Minute amounts of yttrium deposited on a silicon (100) surface assemble into ultrathin YSi₂ nanowires. Ultrathin nanowires receive a great deal of interest due to their possible uses as interconnects in nano electronic devices or as nano-electrodes to measure e.g. the transverse current across DNA molecules in nanofluidic channels. Here we present electrical conductance measurements of a nanowire bridged by macroscopic electrodes and the characterization of the nanowire/ electrode contact by scanning probe microscopy. The stability of the nanowires after exposure to air, water, and a KCl solution is also addressed for future use in nanofluidics. Research was conducted in part at the Center for Nanophase Materials Sciences, sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. DOE.

8:24AM H20.00003 Copper Incorporation into ZnO Nanowires. SUSIE EUSTIS, DOUGLAS MEIER, BABAK NIKOBAKHHT, NIST — The applications of zinc oxide (ZnO) nanowires (NWs) in devices are promising due to the optical, mechanical and electrical properties of these one-dimensional structures, but current uses are limited by the ability to produce high quality nanowires at desired locations. Copper is an attractive catalyst for generating zinc oxide nanowires due to the long length and high density of ZnO NWs produced. However, defects due to impurities, oxygen deficiencies, and structural defects lead to decreased optical and electrical transport. Photoluminescence (PL) microscopy found that ZnO NWs grown by high temperature evaporation on a bulk copper substrate display the expected band gap emission at 380nm. A larger visible emission is also observed in the PL spectrum around 580nm due to defect states. High-resolution transmission electron microscopy (HR-TEM) shows the ZnO nanowires are single crystalline with hexagonal structure. The metallic tip shows a polycrystalline structure in HR-TEM images. Energy dispersive x-ray spectroscopy (EDS) mapping and auger electron spectroscopy (AES) clearly show copper throughout the length of the nanowire, which is most likely responsible for the strong deep trap emission from these nanowires. AES also finds large amounts of oxygen on the surface of these NWs, a further contributor to defect emission states.
8:36AM H20.00004 Self-organization of atom wires on vicinal surfaces 1

Paul Snijders, Oak Ridge National Laboratory — Self-organization is possibly the best way to produce nanostructures in large quantities. This also holds for the ultimate 1D system, atom wires; they can be self-assembled in large arrays on vicinal Si surfaces. Such atom wire systems often show intriguing electronic properties such as competing charge density waves and spin-orbit split one-dimensional bands. However, because of their low dimensionality, these wires also frequently show profound thermodynamic fluctuations that limit their structural uniformity and have a large influence on their electronic properties. Therefore, in this talk I will focus on structural fluctuations in Ga atom wires self-organized on the Si(112) surface. In these atom wires, strain-relieving adatom vacancies self-organize into meandering vacancy lines (VLs) similar to the well-known nx2 superstructures for Ge on Si(100). The average spacing between these line defects can be experimentally controlled continuously by adjusting the chemical potential $\mu$ of the Ga adatoms. Significant VL correlations are discovered in STM experiments that cannot be captured within a mean field analysis. These structural fluctuations are well described by a new lattice model that combines Density Functional Theory (DFT) calculations for perfectly ordered structures with the fluctuating disorder seen in experiment, and the experimental control parameter $\mu$. This hybrid approach of lattice modeling and DFT can be applied to other examples of line defects in hetero-epitaxy, especially in cases where correlation effects are significant and a mean field approach is not valid.

1Part of this work was supported by the US DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, through Oak Ridge National Laboratory which is managed by UT-Battelle, LLC.

9:12AM H20.00005 Growth and Properties of Self-Aligned MgO Nanowires

Elena Cimpoiasu, Dept. of Physics, United States Naval Academy, Annapolis, MD 21402, Robert F. Klue, Dept. of Physics, University of Illinois at Chicago, Chicago, IL 60657, Ryan A. Mundie, Dept. of Applied Physics, Yale University, New Haven, CT 06520, Mark A. Reed, Depts. of Electrical Engineering and Applied Physics, Yale University, New Haven, CT 06520 — A simple VLS route was used to produce self-aligned MgO nanowires on both polished crystalline (c-axis sapphire) and ceramic (alumina) surfaces. Growth on alumina produces vertically-aligned, very thin nanowires, indicating enhanced growth at the liquid-solid interface. Growth on polished sapphire results in faceted MgO nanowires which are perpendicular to the r-plane of sapphire and show evidence of competing vapor-solid-growth mechanism. The difference in the morphology and structure of the nanowires growing on the two different substrates clearly illustrates the affect of substrate on the growth process. This work was partially supported by DARPA, by the Department of Homeland Security, and by the National Science Foundation.

9:24AM H20.00006 Novel Nanocomposites for Energy and Electromagnetic Applications via 3D self-assembly 1

Amit Goyal, Sung-Hun Wee, Yanfei Gao, Junsou Shin, Karren More, Yuri Zuev, Claudia Canton, Jianxin Zhong, Malcolm Stocks, Oak Ridge National Laboratory — Nanocomposites comprising ordered 3D arrays of nanodots of one type of ceramic material coherently embedded in another ceramic matrix comprise are expected to exhibit novel physical properties tunable by adjusting the overall composition, concentration, feature size and spatial ordering of the nanodots. Wide-ranging applications such as photovoltaics, solid state lighting, ultra-high density storage and high temperature superconductivity are of interest. We report here on a joint experimental, theoretical and computational study on achieving 3D ordering via 3D self-assembly of nanodots of a complex ceramic material within another complex ceramic material, such as 3D self-assembly of BaZrO3 nanodots in REBCO superconducting films. Examples will also be given for other ceramic and metal/ceramic systems. In all cases 3D self-assembly was obtained in epitaxial thick films grown via pulsed laser ablation on single-crystal or single-crystal-like substrates.

Research was sponsored by the U.S. Department of Energy under contract DE-AC05-00OR22725 and by an internal Laboratory Directed Research & Development (LDRD) project.

9:36AM H20.00007 Terrace-width Distributions on Vicinal Surfaces: Effective Attraction Between Noninteracting Touching Steps 1

Rajesh Sathiyarayanan, Ajimi Bhadja Hammouda, T.L. Einstein, University of Maryland, College Park — Terrace-width distributions (TWDs) characterize equilibrium as well as non-equilibrium morphology of vicinal surfaces. Using the terrace-step-kink (TSK) model, we apply Monte Carlo simulations (both Metropolis and kinetic) to study TWDs. Steps interact via inverse-square entropic and elastic interactions. Steps cannot touch each other (except at corners) have monatomic height; their configurations, correspond to the worldlines of fermions in 1D. The associated TWDs are well described by the generalized Wigner surmise. The fit parameter $\gamma$ is directly related to the dimensionless energetic interaction strength $A[\gamma]$ if steps are allowed to touch, one can find some double (or greater) height steps. For closely spaced steps, this can alter the TWD considerably. We simulated the TWD of steps with $A = 0$ but touching allowed. Our results indicate an effective attraction between steps, as reflected by a value of $\gamma$ significantly less than 2 (the $A = 0$ value with touching forbidden). As expected, this effective attraction becomes weaker as the terraces become wider; we discuss the crossover behavior.

1Supported by NSF MRSEC Grant DMR 05-20471


9:48AM H20.00008 Study of Fe atomic chains on Pt(997) vicinal surface

Elijah Ayieta, Indiana University—Purdue Uni, Ya.B Losovyi, LSU, Cheng Ruihua, IUPUI — The vicinal substrates form the promising templates for low cost effective bottom-up fabrications of nanostructures. A variety of one-dimensional atomic chains can be synthesized on the stepped surfaces. The electronic structure of a vicinal surface plays a significant role in determining the physical properties of atomic chains on stepped surface as well as the surface morphology. The Pt(997) surface is cut 6.5° of Pt(111) surface forming terrace width of 2nm. The surface of the substrate is then characterized using scanning tunneling microscopy STM and angle resolved photoemission spectroscopy from synchrotron radiation source. The data shows that the surface has uniform steps with no reconstructions. Electron confinement is observed with wave vector perpendicular to the step direction. Fe atomic chains were then carefully deposited on the surface of Pt(997) and then finally characterized. The exchange splitting of Fe 3d bands is estimated according to the photoemission spectroscopy data.

10:00AM H20.00009 Thermoelectric properties of Bi2Te3 films and nanowire arrays

Cheng Lung Chen, Yang Yuan Chen, P. C. Lee, C. T. Chen, S. R. Harutyunyan, S. J. Lai, C. D. Chen, S. J. Lin, Institute of Physics, Academia Sinica Team — The n-type Bi2Te3 nanowire arrays with diameter ~120 nm and thin films with thickness ~10 μm have been fabricated by electrochemical deposition from nitric acid bath, containing bismuth nitrate and tellurium dioxide. Extensive characterizations of the morphology, structure, and composition of the films and nanowires were performed by means of SEM, XRD, EDS, and TEM. The films have nanocrystalline structure whereas the nanowires are single crystallines. The influence of microstructure on thermoelectric properties was investigated by comparison charge carrier transport in two mutually perpendicular crystallographic directions. The measurements of Seebeck coefficient and electrical resistivity were carried out in temperature region of 180 to 300 K. The highest value of $\sigma^2 = 840 \text{TW/m·K}^2$ was obtained at 285 K for film. The electrical resistivity of an individual Bi2Te3 nanowire is ~4.3 μΩ·m using e-beam lithography technique. Based on the Seebeck coefficient obtained from nanowire arrays, the calculated value of $\sigma^2$ for single nanowire is ~1000 μWm·K−2 which is higher than that of the film. These results may help in designing processes for thermoelectric microdevices.
STM images will be presented and a detailed analysis of the electronic structure of all the proposed structures will be discussed.

formed by single or pair of atoms; and the first layer may be commensurate or incommensurate with the substrate. Comparison between calculated and observed

From the theoretical side, we propose several structures of Si on Ag(110) where Si atoms occupy either single or double layers, with the second layer may be

wires 5 lattice constants wide, we observed 4 distinct bright spots across the wire with a periodicity of 2 times the Ag nearest neighbor distance along the wire.

Universite de Cergy, France, G. LELAY, B. AUFRAY, CRMCN-CNRS, Luminy, France — Si nanowires images on Ag(110) were obtained using Scanning

studies

multi-component alloys provide a natural means of tuning the band gap and other parameters to optimize and extend the application of semiconductor elec-

conducting nanowires.

Curved tips have been observed at one end of the nanowires which contain same elemental components as the body of the nanowires. This technique is proven

to be a successful approach to eliminate the need for external catalyst which can have detrimental consequences affecting the performance of an optoelectronic
device. As-synthesized nanowires were characterized using TEM, SEM, XRD, EDS, photo luminescence, Vis-IR absorption and Raman spectroscopy. Results of transport properties of individual nanowires will also be presented.

10:36AM H20.00012 Low melting metal-induced synthesis of multi-component III-V semi-

conducting nanowires. , ROMANEH JALILIAN, ZHIQIANG CHEN, GAMINI SUMANASEKERA, University of Louisville — Semiconductor multi-component alloys provide a natural means of tuning the band gap and other parameters to optimize and extend the application of semiconductor electronic/optoelectronic devices. In this study, multi-component nanowires have been synthesized in vapor phase by laser ablation of solid targets consisting of initial bulk materials. Growth of nano-crystals is believed to seed from low melting metallic droplets generated from laser bombardment and heating of the target. Curved tips have been observed at one end of the nanowires which contain same elemental components as the body of the nanowires. This technique is proven to be a successful approach to eliminate the need for external catalyst which can have detrimental consequences affecting the performance of an optoelectronic device. As-synthesized nanowires were characterized using TEM, SEM, XRD, EDS, photo luminescence, Vis-IR absorption and Raman spectroscopy. Results of transport properties of individual nanowires will also be presented.

Si nanowires on Ag(110): an experimental and electronic structure studies1 , A. KARA, Department of Physics, University of Central Florida, B. EALET, C. LEANDRI, CRMCN-CNRS, Luminy, France, H. OUGHADDOU, Universite de Cergy, France, G. LEILAY, B. AUFRAY, CRMCN-CNRS, Luminy, France — Si nanowires images on Ag(110) were obtained using Scanning Tunneling Microscopy. Wires with tailored width and very large lengths were observed with the wires growing along the open channels of Ag(110). For those wires 5 lattice constants wide, we observed 4 distinct bright spots across the wire with a periodicity of 2 times the Ag nearest neighbor distance along the wire. From the theoretical side, we propose several structures of Si on Ag(110) where Si atoms occupy either single or double layers, with the second layer may be formed by single or pair of atoms; and the first layer may be commensurate or incommensurate with the substrate. Comparison between calculated and observed STM images will be presented and a detailed analysis of the electronic structure of all the proposed structures will be discussed.

1 Computational work done at NCSA grant # TG-DMR070006T.

Tuesday, March 11, 2008 8:00AM - 10:48AM — Session H21 DCP: Focus Session: Clusters, Cluster Assemblies, Nanoscale Materials III Morial Convention Center 213

8:00AM H21.00001 Probing electronic and magnetic properties of atomic and molecular clusters with sharp tips1 , JEAN-PIERRE BUCHER, Université LouisPasteur, Institut de Physique et Chimie des Matériaux de Strasbourg — Probing magnetic and transport properties on a local basis with the tip of a scanning tunneling microscope (STM) allows establishing close links with the exciting field of magnetic read and write processes. Some examples of applications of this approach to magnetic nanostructures will be shown. First of all, the fundamental properties of Co nanoclusters, on metal surfaces will be presented. These clusters have been probed by low temperature dl/dV spectroscopy (STS). It is found that occupied electronic surface states of the Co clusters are sensitive to the crystallographic stacking and furthermore exhibit a downward energy shift as the cluster size decreases. Ab initio calculations confirm that the observed shift is due to the size dependent mesoscopic relaxation in the clusters. When a magnetic tip is used in low temperature spin polarized (SP)-STM experiment, it is possible to reveal spin polarized feature in the local density of states. For example, one is able to identify two magnetization states of the nanometer Co clusters, corresponding to the parallel or antiparallel configuration with respect to the tip polarization. Progress in the emerging field of spintronics strongly relies on the fundamental understanding of electron/spin transport and magnetic phenomena in reduced dimensions, down to the extreme limit of individual molecules, or even single atoms where sizeable quantum effects are expected. Electronic and magnetic properties of Co atoms and metal-based molecular magnets adsorbed on magnetic nano-islands or on non magnetic surfaces will be presented. On the example of Co-pherrocyanines prepared in UHV at 4.6 K, it will be shown that dl/dV characteristics are representative of both, the nature of the molecule and also its interaction with the substrate.

1 Support from the MAGMANet network of excellence of the European Community is greatly acknowledged.

8:36AM H21.00002 First Principles Theory of Supported Clusters with Complex Magnetic Order. , OLLE ERIKSSON, Uppsala University — It is demonstrated that the magnetic interactions can be drastically different for nano-sized systems compared to those of bulk or surfaces. In a real-space formalism we have developed a technique to calculate non-collinear magnetization structures and hence exchange interactions. Our results for magnetic Cr, Mn and Fe clusters supported on a Cu(111) surface show that the magnetic ordering as a rule is non-collinear and can not always be described using a simple Heisenberg Hamiltonian. We argue that the use of ab initio calculations allowing for non-collinear coupling between atomic spins constitute an efficient and reliable way of analyzing nano-sized magnets.
9:12AM H21.00003 Magnetic properties and stability of mettalloinorganic clusters1, ROBERTO ROBLES, SHIV KHANNA, Dept. of Physics, Virginia Commonwealth University, Richmond, VA 23284 — Theoretical studies on the structure, stability, electronic structure and magnetic properties of binary clusters Si,TMg (n=1-8, TM=Cr,Mn) have been carried out within a density functional formalism using the generalized gradient approximation. The stability of the clusters as a function size is analyzed in terms of several criteria, like the progression in bonding energy and HOMO-LUMO gap, with the ultimate objective of identifying the simple rules that can guide the search of stable species. The magnetic properties of the clusters are investigated by considering different ferromagnetic and antiferromagnetic arrangements of the local spin moments and optimizing the geometry and the spin state to determine the ground state including possible isomers. The possible use of these clusters as building blocks of cluster assemblies is discussed, and finally, the interest of these assemblies in the design of materials which could be used in the field of spintronics is briefly considered.

1We are grateful to U.S. Department for financial support (MURI Grant # W911NF-06-1-0280).

9:24AM H21.00004 Intermediate valence, local antiferromagnetic coupling and the Kondo effect in ytterbium organometallic molecules, C.H. BOOTH, R.W. LUKENS, Lawrence Berkeley National Laboratory (LBNL), M.D. WALTER, D. KAZHDAN, K.A. ANDERSEN, LBNL and University of California, Berkeley, E.D. BAUER, Los Alamos National Laboratory, L. MARON, INS A Toulouse, O. EISENSTEIN, Universite Montpellier — Studying magnetic ions coupling to aromatic rings in organometallic molecules provides an analogous route to studying the Kondo effect in nanoscale systems. We extend the number of molecules displaying such effects in their magnetism and X-ray absorption spectroscopy from cerocene [Ce(Cp₃H₅)₂] and Cp*Yb(bipy) [Cp* = pentamethylcyclopentadienyl, bipy = bipyridine] to a collection of Cp*₃Yb(L) molecules, where L is one of various bipyridyl or diazadiene ligands. Clear trends are observed in both the magnetic susceptibility and the Yb valence that indicate changes in the fundamental temperature scale. CASSCF calculations indicate the intermediate valence is primarily due to a configuration interaction between the open-shell f₁₃/₂₋₁ and the closed-shell f₁₄/₂₋₁ spin-singlet states, in direct analogy to the Kondo effect in intermetallic systems. These studies increase the range of molecular species where such properties are observed, and point toward understanding the ubiquity of such effects and their involvement in fundamental bonding and magnetism in organometallic molecules.

9:36AM H21.00005 The structure, stability, and magnetic properties of Au(111)/NiO(111) interface: density functional theory study1, K.L. YAO, Y.L. LI, Z.L. LIU, Huazhong University of Science and Technology — We studied the electronic structure of Au(111)/NiO(111) interface in accordance with the two models of NiO(111) surface. The work of adhesion, the spin magnetic moment, the stability and the electronic properties of the Au(111)/NiO(111) interface were calculated by density functional theory (DFT). The calculated results of Au(111)/NiO(111) interface were then compared with non-polar Au(100)/NiO(100) interface. At the same time, the total density of states (DOS) of Au(111)/NiO(111) interface corresponding to the two models were also calculated. The calculations reveal that the Ni-terminated and the oxidized interfaces have antiferromagnetic properties, while the O-terminated interface exhibits ferromagnetic properties.

1This work was supported by the National Natural Science Foundation of China under Grant Nos. 10574047,10574048 and 20490210. It was also supported by National 973 project under grant No. 2006CB921600.

9:48AM H21.00006 Investigating the Molecular Level Details of Catalytic Oxidation Reactions1, GRANT JOHNSON, Pennsylvania State University — Gas-phase cluster reactivity studies are providing significant insight into the molecular level mechanisms of oxidation reactions occurring on catalytic surfaces. Our experimental approach, employing tandem mass spectrometry, uses mass selected metal oxide clusters to model specific catalytic active sites. This technique enables investigation of the influence of factors such as size, stoichiometry, charge state, and elemental composition on the reactivity of catalytic materials. Particular emphasis is on identifying species with enhanced activity for the selective oxidation of simple hydrocarbons and atmospheric pollutants. Recent findings pertain to the kinetics of ethylene oxidation in the presence of vanadium oxides and the oxidation of carbon monoxide in the presence of gold and iron. Through a combination of experiments and theoretical calculations we establish structure-reactivity relationships and propose general reaction mechanisms for these catalytic processes.

1Financial support provided by the U. S. Department of Energy, Grant No. DE-FG02-92ER14258.

10:24AM H21.00007 Effect of ligand on the geometric and electronic structure of Au₁₃ cluster1, GHAZAL SHAFAI, SAMPYO HONG, TALAT RAHMAN, University of Central Florida, MASSIMO BERTINO, Virginia Commonwealth University — We have carried out calculations based on the density functional theory in the projector augmented wave scheme (PAW) and the pseudopotential approach, to examine the effect of the ligand on the geometric and electronic structure of Au₁₃ cluster. We find bare Au₁₃ to form a flat flake, in agreement with previous theoretical calculations. This structure is lower in energy by 2.60 eV in comparison with the well ordered icosahedron geometry. Our results show, however, that the Au₁₃ cluster covered with ligands of phosphine (PH₃) forms a stable spherical structure (icosahedron) in agreement with the experiment [1] which is by 0.08 eV lower in energy when compared to the flatflake complex. If the phosphine is replaced by H, the well ordered icosahedron structure is no longer stable, but it still maintains a 3 dimensional form, signifying the effect of the ligand in stabilization of the structure. We observe a narrow d-band for flat-flake gold atoms in the complex, while in the icosahedron structure the d-band is wider. We also find a stronger overlap between the p orbitals of the P atom with d orbitals of gold atoms in the icosahedron complex. [1] M. F. Bertino et. al. Phys. Chem. B Lett. 110, 21416 (2006)

1Work supported in part by DOE grant DE-FG02-03ER46354.

10:36AM H21.00008 Superheating, Melting and Precursors to Melting in Metal Nanoparticles, DIMITRI SCHEBARCHOV, Victoria University of Wellington, SHAUN HENDY, Industrial Research Ltd — We have investigated precursors to melting in metal nanoparticles using molecular dynamics in the microcanonical ensemble. At the onset of solid-liquid phase coexistence, we find first-order transitions in clusters of non-melting facets (i.e. facets that are not wet by the melt such as Pb (111)), and continuous transitions otherwise. In sufficiently small clusters however, we find that static solid-liquid coexistence is unstable. Further, the size at which the instability arises, and even the melting temperature, depends on the ability of the melt to wet the solid facets of the cluster. In particles with non-melting facets we show that the melting temperature can exceed that of the bulk material. Finally, we also discuss a range of solid-solid transitions that have been observed to occur during solid-liquid phase coexistence, some of which are again driven by the preference of the melt to wet certain crystal facets.

Tuesday, March 11, 2008 8:00AM - 10:36AM – Session H22 DPOLY: Electrically and Optically Active Polymers – Morial Convention Center 214

8:00AM H22.00001 Polymer Physics Prize Break –
8:36 AM H22.00002 Periodic Polymers for Technology, Edwin Thomas, M.I.T. — Periodic polymeric materials comprised of solid polymer and air have interesting interactions with electromagnetic and mechanical waves giving rise to complex dispersion relations including zero density of states (band gaps). The key concern for photonic materials is dielectric contrast, whereas for phononic materials, it is density contrast and relative speed of longitudinal and transverse waves in the two media that is important. The creation of a material with a dual band gap, that is a complete band gap for light and a complete band gap for sound would allow strong coupling in localized defect regions. Progress in this area requires the ability to design and model targeted geometries and excellent control of structure fabrication. Top-down, and bottom-up approaches, involving interference lithography and self-assembly respectively are demonstrating good success in fabricating the requisite structures and creating desired properties for photonics and phononics.

8:48 AM H22.00003 First-principles investigation of high energy density in PVDF copolymers, V. Ranjan, Liping Lu, NC State U., Raleigh, Michael Bongiorno Nardelli, J. Bernholdt, NC State U., Raleigh and ORNL, TN — PVDF and its copolymers exhibit excellent electromechanical properties and in the case of PVDF-CTFE also a very high energy density [1]. We have investigated the phase diagram of these systems and can quantitatively explain the observed energy density of PVDF-CTFE as due to a para to ferroelectric phase transition in a disordered, multidomain structure [2]. Our results show that pure PVDF prefers the α phase at zero field. Electric field lowers the free energy of the β phase, resulting in a structural phase transition at a sufficiently high field. Copolymer admixture lowers the critical field and eventually leads to an energetic preference for the β phase even at zero field. For PVDF-CTFE with CTFE content below 17 %, the α phase is still preferred and the field-induced phase transformation reversibly stores large amounts of energy. For PVDF-TeF, the total energy difference between the two phases is much smaller, resulting in substantially smaller energy density. [1] B. Chu et al., Science 313, 334 (2006). [2] V. Ranjan et al., PRL 99, 047801 (2007).

9:00 AM H22.00004 High and Stable Light Induced Birefringence from Spacer-Free Dye-Polyelectrolyte Liquid Crystal Complexes, Qian Zhang, C. Geraldine Bazuin, University of Montreal, Christopher J. Barrett, McGill University, Christian Pellerin, University of Montreal — Azo materials are promising in photonic applications due to the well-known photoisomerization of azo groups, which, for example, allows efficient inscription of gratings using light induced birefringence (LIB). The incorporation of liquid crystal (LC) character in these materials can be desirable to improve LIB properties, such as in side chain liquid crystal polymers (SCLCPs). However, SCLCPs are costly, and flexible alkyl spacers tend to diminish LIB properties. Here, we present LC azo materials obtained by simple ionic polymerization procedures involving commercially available (or easily synthesized) dyes and oppositely charged polyelectrolytes; for example, methyl orange (MO) and methylated poly(4-vinyl pyridine) (PVPMe). The latter complex, which possesses neither flexible spacer nor tail, has a single-layer smectic A-like structure until degradation and provides exceptionally high and stable LIB properties. These materials can be inscribed with surface relief gratings. Moreover, we have successfully obtained a photoresponsive electrospun mat from a solution of the MO/PVPMe complex mixed with poly(ethylene oxide).

9:12 AM H22.00005 Reducing radiation-induced conductivity in polymeric dielectrics by small molecule electron traps, Robert J. Klein, John L. Schroeder, Shannon M. Lacy, Michael E. Belcher, Phillip J. Cole, Joseph L. Lenhart, Sandia National Laboratories — Polymeric dielectrics, when exposed to ionizing radiation, undergo the formation of electron-hole pairs and consequently exhibit radiation-induced conductivity (RIC), severely limiting the insulating capability of polymeric dielectrics used in ionizing environments. RIC can be significantly reduced by the incorporation of small-molecule traps: in the appropriate concentration range, small molecules consisting of aromatic rings and strongly electron-withdrawing groups can reduce RIC by more than 95 % in poly(ethylene terephthalate) films. The dopant structure is critical: the addition of one nitro group, the strongest electron-withdrawing substituent, leads to > 98 % RIC reduction when placed on fluorenone, pyrene, acenaphthene, and anthracene cores. Other substituents, such as cyano or amino, improve RIC reduction over the isolated cores, but not as effectively as the nitro group. The electron-withdrawing capability of each substituent side group can be quantified using the Hammett parameter.

9:24 AM H22.00006 Dynamics of acoustic phonons in exciton self-trapping in a quasi-one-dimensional system, F.X. Morrissey, S.L. Dexheimer, Washington State University — The localization of electronic excitations via electron-lattice interactions is an important fundamental process in molecular-based electronic materials. In our previous work, we directly time-resolved the electronic and vibrational dynamics of the exciton self-trapping process in the quasi-one-dimensional mixed-valence metal-halide linear chain (MX) complexes [Pt(en)2]2[Pt(en)2]2X2, (X = Cl, Br, I) using femtosecond coherent phonon techniques. In this work, we present transient absorption measurements on PtBr(en) at low temperature that reveal a large amplitude, strongly damped oscillatory component at a frequency of 11 cm−1 that is consistent with the generation of a coherent acoustic wave associated with the formation of the localized lattice deformation that stabilizes the self-trapped state. Comparison with models for polaron formation provides an estimate of the spatial extent of the local deformation of ~ 5 unit cells. This work is supported by the NSF under grant DMR-0305403.

9:36 AM H22.00007 THz time domain spectroscopy of low-frequency vibrations in a quasi-one-dimensional system, A. Bandypadhyay, S.L. Dexheimer, Washington State University — The mixed-valence halide-bridged transition metal linear chain (MX) complexes are prototypical quasi-one-dimensional systems, with a charge density wave ground state and localized electronic excitations analogous to those of conjugated organic polymers. In this work, we present studies of the low-frequency infrared-active vibrational modes of the MX complex [Pt(ethbylendiamine)2]2[Pt(ethbylendiamine)2]2[PF6]2 in the frequency range 0.3 - 3 THz using terahertz time-domain spectroscopic techniques. Distinct polarization-dependent complex refractive indices are observed in single-crystal samples of this highly anisotropic material. The measurements reveal a strong absorption at a frequency of 2.24 THz (75 cm−1) polarized along the chain axis, which we assign to the infrared-active ω1 vibrational mode, involving relative motion of the mixed-valence ions in the charge density wave configuration. This work is supported by NSF grant DMR-0706407.

9:48 AM H22.00008 Optical studies of Pt-rich π-conjugated Polymers, Tomer Drori, M. Tong, A. Gambetti, S. Singh, C. Yang, Z. V. Vardeny, Physics Department, University of Utah, S. Tretiak, Theoretical Division, LANL, Los Alamos — We have used a variety of steady state and ultrafast spectroscopies for studying the photophysics of platinum-containing conjugated polymers, which have potential applications as the active layer of light-emitting diodes. The heavy metal Pt atom that is incorporated in the polymer chain dramatically increases the spin-orbit coupling, and this influences both the intersystem crossing time, T1, and the phosphorescence emission intensity. The Pt-polymers were newly synthesized, where the intrachain Pt atom was incorporated into the polymer either in each (Pt-1) or in every three (Pt-3) monomer units. We will discuss an interesting effect for the photoexcited triplets, which dramatically influence the phosphorescence spectral shape vs. temperature. We also observed the existence of circular polarization memory of the phosphorescence emission in Pt-1 polymers, in which the platinum atoms are separated by only one phenyl ring; but not in Pt-3.

3Acknowledgements: CSACS/CRMA, NSERC Canada, FQRNT Quebec
Improving the Morphology of As-Deposited Films

relatively shallow absorption depths and a high local density of vibrational excitation. The data and model are consistent with a steady-state ablation mechanism, modified by plume shielding late in the microseconds-long FEL functions of individual C-H and C-C bonds with the spectral profile of the picosecond FEL micropulses. Data from ablation rate, ablation depth, time-resolved free-electron laser (FEL) with an unusual micropulse-macropulse temporal structure. We have fully characterized the resonant and non-resonant IR ablation the IR excitation of complex polymer materials is poorly understood, and partly because most of the experiments have been conducted with a tunable infrared the ablation of intact polymers by resonant infrared (IR) laser irradiation has been demonstrated, the mechanism has remained mysterious. This is partly because lasers naturally pump and probe vibrational transitions, but it is also useful to think of vibrational energy as being conducted from one location in a molecule to another. We have developed a new technique where energy is driven into a specific part of molecules adsorbed on a metal surface, and ultrafast nonlinear coherent vibrational spectroscopy is used to watch the energy arrive at another part. This technique is the analog of a flash thermal conductance apparatus, except it probes energy flow with angstrom spatial and femtosecond temporal resolution. Specific examples to be presented include energy flow along alkane chains, and energy flow into substituted benzenes. Ref: Z. Wang, J. A. Carter, A. Lagutchev, Y. K. Koh, N.-H. Seong, D. G. Cahill, and D. D. Dlott, Ultrafast flash thermal conductance of molecular chains, Science 317, 787-790 (2007).


perennial problem in chemical physics. Usually vibrational energy dynamics are viewed through the lens of time-dependent level populations. This is natural because lasers naturally pump and probe vibrational transitions, but it is also useful to think of vibrational energy as being conducted from one location in a molecule to another. We have developed a new technique where energy is driven into a specific part of molecules adsorbed on a metal surface, and ultrafast nonlinear coherent vibrational spectroscopy is used to watch the energy arrive at another part. This technique is the analog of a flash thermal conductance apparatus, except it probes energy flow with angstrom spatial and femtosecond temporal resolution. Specific examples to be presented include energy flow along alkane chains, and energy flow into substituted benzenes. Ref: Z. Wang, J. A. Carter, A. Lagutchev, Y. K. Koh, N.-H. Seong, D. G. Cahill, and D. D. Dlott, Ultrafast flash thermal conductance of molecular chains, Science 317, 787-790 (2007).

This material is based upon work supported by the National Science Foundation under award DMR 0504038 and the Air Force Office of Scientific Research under award FA9550-06-1-0235.

Mechanism of Resonant Infrared Laser Ablation of Polystyrene. — STEPHEN JOHNSON, RICHARD HAGLUND, Vanderbilt University, DANIEL BUBB, Rutgers University, Camden, KANNÄSSEN APPIWOO, Berea College — Although the ablation of intact polymers by resonant infrared (IR) laser irradiation has been demonstrated, the mechanism has remained mysterious. This is partly because the IR excitation of complex polymer materials is poorly understood, and partly because most of the experiments have been conducted with a tunable infrared free-electron laser (FEL) with an unusual micropulse-macropulse temporal structure. We have fully characterized the resonant and non-resonant IR ablation of polystyrene (PS) at several IR wavelengths. The energy input at each wavelength was ascertained by convoluting the temperature-corrected lineshape functions of individual C-H and C-C bonds with the spectral profile of the picosecond FEL micropulses. Data from ablation rate, ablation depth, time-resolved photoacoustic and photothermal measurements and nanosecond pulsed-laser shadowgraphy were fed into a simple finite-element model of energy deposition and relaxation. The data and model are consistent with a steady-state ablation mechanism, modified by plume shielding late in the microseconds-long FEL macropulse. Thus the mechanism of the resonant IR laser ablation process is apparently connected primarily with the bond-selective absorption leading to relatively shallow absorption depths and a high local density of vibrational excitation.

Support is acknowledged from NSF Grant number CMMI-0727713.
9:00AM H23.00004 Laser Ablation Electrospray Ionization: A Molecular Probe for Biological Tissues, PETER VEMES, ALEXIS A. BARTON, YUE LI, AKOS VERTES, George Washington University — Interaction of light and matter has long served as the basis of probing and modifying physical and chemical properties of materials. Recent biomedical applications focus on the mid-infrared (mid-IR) region to couple the laser energy into samples through absorption by the native water. For example, mass spectrometry (MS), relying on atmospheric pressure mid-IR matrix-assisted laser desorption ionization, takes advantage of the small amount of ions in the laser plume. In mid-IR laser ablation, owing to the recoil pressure buildup in the sample, most of the material is expelled in the form of neutral molecules, clusters, and particulates. To enhance ion production, we intercept this plume with a cloud of charged droplets to post-ionize them for MS. As a result, laser ablation electrospray ionization (LAESI) can directly probe the molecular makeup of water-rich targets with superior ion yield and dramatically extended mass range (up to 66,500 m/z). LAESI also enables two and three dimensional imaging of live tissues. Fast imaging of the plume-plume interaction reveals the mechanistic aspects of LAESI.

9:12AM H23.00005 Deposition of functional nanoparticle thin films by resonant infrared laser ablation, RICHARD HAGLUND, STEPHEN JOHNSON, Vanderbilt University, HEE K. PARK, AppliFlex LLC, KANNATESSEN APPAVOO, Berea College — We have deposited thin films containing functional nanoparticles, using tunable infrared light from a picosecond free-electron laser (FEL). Thin films of the green light-emitting molecule Alq3 were first deposited by resonant infrared laser ablation at 6.68 μm, targeting the C=C ring mode of the Alq3. TiO2 nanoparticles 50-100 nm diameter were then suspended in a water matrix, frozen, and transferred by resonant infrared laser ablation at 2.94 μm through a shadow mask onto the Alq3 film. Photoluminescence was substantially enhanced in the regions of the film covered by the TiO2 nanoparticles. In a second experiment, gold nanoparticles with diameters in the range of 50-100 nm were suspended in the conducting polymer and anti-static coating material PEDOT:PSS, which was diluted with mixing with N-methyl pyrroldinone (NMP). The gold nanoparticle concentration was 8-10% by weight. The mixture was frozen and then ablated by tuning the FEL to 3.47 μm, the C-H stretch mode of NMP. Optical spectroscopy of the thin film deposited by resonant infrared laser ablation exhibited the surface-plasmon resonance characteristic of the Au nanoparticles. These experiments illustrate the versatility of matrix-assisted resonant infrared laser ablation as a technique for depositing thin films containing functionalized nanoparticles.

9:24AM H23.00006 Photochemical ablation of Polytetrafluoroethylene (PTFE) under 157-nm irradiation, SHARON R. JOHN, STEVEN C. LANGFORD, J. THOMAS DICKINSON, Washington State University — We report time- and mass-resolved measurements on neutral molecular particles emitted from polytetrafluoroethylene during exposure to 157-nm laser radiation at fluxes where relative rapid etching is observed. By comparing the time-of-flight signals from a range of masses, we conclude that (CF2)N fragments for N=1-6 are emitted directly from the surface in substantial quantities. In contrast, the monomer (N=2) is the principal product during irradiation at 248 nm, due to a thermal decomposition mechanism. The time-of-flight signals of all the (CF2)N fragments show fast components with kinetic energies of ~0.6 eV, indicating a non-thermal mechanism. These high kinetic energies are consistent with photochemical scission of the polymer backbone, where a part of the excitation energy is delivered to the fragment as kinetic energy. Although clean etching is observed under these conditions, the great majority of the mass removed appears as much larger fragments with a size distribution of 10 nm to 1 μm. The time-of-flight signals also show a slow component. We present a collisional model to explain the slowing down of neutrals molecules created by photochemical scission. Intense electron, positive and negative ion emissions are also observed. Their formation and emission mechanism will be discussed.

9:36AM H23.00007 Rational Design of Two-Photon Absorbing Photographic Materials for Optical Switching and Data Storage1, I.A. MIKHAILOV, K.D. BELFIELD, A.E. MASUNOV, University of Central Florida — Diarylenes are able to undergo light-induced transition from the open to closed ring isomer (photoisomerization) accompanied by the change in optical properties (photochromism). This ability holds a great promise for photonic applications, including optical data storage and ultrafast optical switching. Photoisomerization initiated by absorption of two photons could drastically increase the density of these devices. However, attachment of fluorine substituent to diarylethenes increased two-photon absorption cross-section led to the loss of photochromatic activity. Analysis of the Kohn-Sham orbitals reveals that the relaxation of the lowest excited state of diarylethene fragment leads to photoisomerization, while the occupied level of the chromophore substituent generates an excited state below the photoreactive one. To design the molecular switch active in two-photon regime we suggest stabilizing the highest occupied orbital, which can be accomplished by fluorination of the chromophore. We applied time dependent Density Functional Theory to predict potential energy surfaces of excited states and two-photon absorbing profiles. The obtained results are in agreement with the qualitative orbital description.

1Supported by the NSF Grant CCF 0740344, NERC, and UCF I2lab.

9:48AM H23.00008 Toward molecular switches and biochemical detectors employing adaptive femtosecond-scale laser pulses1, ROLAND ALLEN, PETRA SAUER, Texas A&M University — The following topics will be discussed: (1) Photoisomerization of azobenzene, with nuclear motion allowing extra electronic transitions for pulse durations ~ 50 fs. (2) Photoinduced ring-opening in a model dithienylethene. (3) Response of dipicolinic acid to femtosecond-scale laser pulses, including excited states and nuclear motion. Although real applications such as molecular switches and biochemical detectors involve more techniques — with femtosecond-scale laser pulses whose durations, photon energies, fluences, shapes, etc. are tailored for specific applications — we will explain the screening effect with excited carrier density. Fourier Transform analysis shows the bare LO phonon and the lower branch of the LO phonon-plasmon coupled modes (L-). With increasing photocarrier density, the LO phonon response is essentially unaffected, while the L- peak red shifts to the TO phonon limit. Time windowed FT analysis reveals complex carrier density dependent spectral evolution. The coupled-carrier phonon dynamics are discussed in the context of photochemical potential scattering and high field transport.

1This work was supported by the Robert A. Welch Foundation.

10:00AM H23.00009 Ultrafast carrier-phonon dynamics under intense optical excitation of GaAs, AMLAN BASAK, Univ of Pittsburgh, M. HASE, Univ of Tsukuba, M. KITAJIMA, NIMS, Tsukuba, HRVOJE PETEK, Univ of Pittsburgh — We report the response of n-doped GaAs (n = 2×10^18 cm^-3) when excited by an e-h pair density n_exc ~ 10^19–10^20 cm^-3 with a 10 fs laser pulse centered at 400 nm. The experiment is performed in resonant electo-optic sampling geometry. The experiment was performed in reflective electro optic sampling geometry. Coherent LO phonon oscillations are excited through both ultrafast screening of the depletion field and the deformation potential scattering. The time domain signal contains near-instantaneous transient electronic response as well as coupled phonon-plasmon oscillation. The amplitude of reflectivity is sub-linearly possibly indicating saturation of the screening effect with excited carrier density. Fourier Transform analysis shows the bare LO phonon and the lower branch of the LO phonon-plasmon coupled modes (L-). With increasing photocarrier density, the LO phonon response is essentially unaffected, while the L- peak red shifts to the TO phonon limit. Time windowed FT analysis reveals complex carrier density dependent spectral evolution. The coupled-carrier phonon dynamics are discussed in the context of photochemical potential scattering and high field transport.

This work was supported by the Robert A. Welch Foundation.
10:12AM H23.00010 Effect of Hot Electron Pressure in Ultrafast Laser Interaction with Metals, ZHIBIN LIN, LEONID ZHIGILEI. Department of Materials Science and Engineering, University of Virginia — Ultrafast laser irradiation can transiently bring a metal into a highly nonequilibrium state in which the electron temperature can reach thousands of Kelvin while the lattice remains cold. Under these conditions the thermal pressure from the hot conduction electrons can play an important role in defining the initial relaxation dynamics of the irradiated target. In this work, a description of the hot electron pressure due to the presence of the excited electrons is incorporated into a continuum-atomistic computational model combining the molecular dynamic method with the two temperature model. Computer simulations employing this approach are performed for Al, Au, and Ni metal films and bulk targets. The effect of the hot electron pressure on the generations of acoustic phonons in the laser-irradiated metal film will be discussed and compared with existing experimental data. The relative contributions of the hot electron pressure and thermoelastic stresses due to the lattice heating to the dynamics of the irradiated target and spallation/ablation process are discussed based on the results of the computer simulations.

10:24AM H23.00011 Coherent LO phonon self-energy renormalization under high photoexcited carrier densities in Si, ANCA-MONIA CONSTANTINESCU, University of Pittsburgh, MUNEAKI HASE1, University of Tsukuba, MASAHIRO KITAJIMA2, National Institute for Material Science, HRVOJE PETEK, University of Pittsburgh — The study of hot carrier-phonon interaction dynamics is motivated by their influence on optical and electrical properties of semiconductors. Following high-density (10^{19}–10^{20} carriers/cm^3) photoexcitation of Si(001) with 10 fs duration 400 nm laser pulses, the complex self-energy (i.e. frequency and decay rate) of coherent LO phonon (k=0) renormalize due to deformation potential interaction with the photogenerated non-equilibrium plasma. We evaluate the time dependent LO phonon frequency and dephasing time by analyzing the transient electro-optic reflectivity of variously doped Si(100). We measure the coherent LO phonon mode oscillations in the transient reflectivity over a delay time of 6 ps between pump and probe pulses. Varying the pump power from 50 to 5 mW, we observe that the electronic softening of the lattice (i.e. LO phonon frequency change) and the quasi-exponential dephasing time of the phonon depend on the initial photoexcited carrier density.

1Japan
2Tsukuba, Japan

10:36AM H23.00012 Mechanistic study of negative ion emission from single crystal alkali halide surfaces due to pulsed UV laser irradiation, J. T. DICKINSON, Washington State University, KENICHI KIMURA, Research Institute, National Printing Bureau of Japan, Odawara, Kanagawa 256-0816 Japan, S. C. LANGFORD, Department of Physics, Washington State University, Pullman, WA 99164 — We report on extensive measurements of negative alkali ion emission from four alkali halides during exposure to 248-nm pulsed excimer laser radiation at fluences well below the threshold for optical breakdown. A detailed study on the emissions from single crystal KCl shows no evidence for negative halide ions, suggesting that negative alkali ions are not formed by electron attachment to thermally emitted neutral particles. Furthermore, the KCl surface charges positively during laser irradiation (due to electron emission from defects), which would hinder direct emission of negative ions from the surface. We present strong evidence for a negative ion formation mechanism involving double electron attachment to singly charged positive alkali ions. Extension of these measurements to single crystal KBr and to other dielectric materials confirm this mechanism.

3This work was supported by the U. S. Department of Energy

10:48AM H23.00013 Observation of Saturable and Reverse Saturable Absorption in Silver Nanodots, ULLAS GURUDAS, DANIEL BUBB, Rutgers-Camden, THOMAS LIPPERT, SEBASTIAN HEROITH, PSI — Saturable absorption (SA) and reverse saturable absorption (RSA) were observed in Ag nanodots prepared by pulsed laser deposition. The Real [Re \(\chi^{(3)}\)] and Imaginary [Im \(\chi^{(3)}\)] part of the third order nonlinearity of these films are measured as and respectively, using Z-scan technique. The decrease of absorption under strong optical illumination results in a negative Im \(\chi^{(3)}\) at the photon energy used. At higher input irradiance RSA becomes dominant. The transformation from SA to RSA suggests that another nonlinear process takes place and become dominant. To evaluate the recovery time of these nonlinear processes and get an idea about the underlying mechanism, we conducted a degenerate pump-probe experiment with 25 psec, 532 nm laser pulses. The increased \(\chi^{(3)}\) and fast response time of the Ag nanoparticles can be used for optical pulse compressor, optical switching, laser pulse narrowing and protecting optical sensors from intense laser pulses.

3Support from and IEEE supplemental award to NSF Grant DMI-0613837.

Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H24 DMP: Focus Session: Optical Properties of Nanostructures III: Functional Nanowires Morial Convention Center 216

8:00AM H24.00001 Polarized Photoluminescence from Single Wurtzite and Zincblende InP Nanowires, A. MISHRA, L.V. TITOVA, T.B. HOANG, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, Y. KIM, H.J. JOYCE, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We use polarized photoluminescence spectroscopy of single InP nanowires to compare the optical properties of vapor-liquid-solid growth of single zincblende (ZB) and wurtzite (W) nanowires. Since ZB and W nanowires have different symmetries and selection rules, their optical properties should also be different. The emission from single W nanowires is observed to be \(\sim\)80 meV higher than for ZB nanowires. Low temperature polarization measurements show that ZB nanowires are strongly polarized along the nanowire axis, while the W nanowires are polarized perpendicular to the NW axis. The temperature dependence of the ZB and W NW emissions are compared with a bulk InP epiayer. Apart from the 80 meV shift in bandgap, the temperature dependencies are similar.

8Support for this work was provided by NSF (#0701703) and the Australian Research Council.

8:12AM H24.00002 Investigation of the Electronic Structure of GaAs/AlGaAs Core Multi-Shell Nanowires, S. PERERA, M.A. FICKENSCHER, T.B. HOANG, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, H.J. JOYCE, Q. GAO, Y. KIM, H.H. TAN, C. JAGADISH, Australian National University — We use photoluminescence and PL excitation spectroscopy to study the electronic structure of GaAs/AlGaAs core multi-shell NWs. Using Au-catalyst assisted MOVD, a 10 nm GaAs quantum well tube (QWT) with AlGaAs barriers is formed surrounding a central \(\sim\)50 nm GaAs core. With resonant excitation at 780 nm emission is seen from both the core as well as the QWT. The QWT emits in a narrow intense peak \(-\)22 meV above the exciton emission from the core suggesting quantum confinement in a 10 nm quantum well. NWs with QW at 100 nm InGaAs core grown shows a similar peak at \(\sim\)100 ns as recombination lifetime, while the core decays in \(\sim\)1 ns. Preliminary PLE measurements exhibit possible excited state structure of this novel quantum-confined nanostructure.

1Support for this work was provided by NSF (#0701703) and the Australian Research Council.
8:24AM H24.00003 Photoluminescence Dynamics of GaAs/AlGaAs Core-Shell Nanowires1
H.J. JOYCE, Y. KIM, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, M.A. FICKENSCHER, S. PERERA, T.B. HOANG, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, X. ZHANG, J. ZOU, University of Queensland — We use time-resolved PL spectroscopy to study the excitation dynamics of GaAs/AlGaAs core-shell nanowires (NWs) at 20 K. NWs were prepared by Au catalyst-assisted MOCVD. PL emission from single NWs exhibits an excitonic peak at ~1.515 eV. The exciton lifetime depends on the morphology and crystallographic defect density of the GaAs core, which are in turn dependent upon the growth conditions. Nanowires cores grow at higher temperatures (450 °C) give short exciton lifetimes (<100 ps). Reducing defects within the nanowire (twinning) or at the interface should increase exciton lifetime and improve luminescence efficiency. Indeed, twin-free minimally tapered nanowires achieved using a low growth temperature (375 °C), exhibit high quantum efficiency with an exciton lifetime approaching 1.6 ns at 20 K.

1Support for this work was provided by NSF (#0701703) and the Australian Research Council.

8:36AM H24.00004 Ultrafast dynamics in semiconductor nanowires, ROHIT PRASANKUMAR, SUGKEUN CHOI, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, GEORGE WANG, Sandia National Laboratories, SAMUEL PICRAUX, ANTOINETTE TAYLOR, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Semiconductor nanowires (NW) have recently attracted much interest due to their novel electronic and optical properties along with their potential for device applications in areas including nanoscale lasers and thermoelectrics. However, the further development and optimization of NW-based devices will depend critically on an understanding of carrier relaxation in these unique nanostructures. Here, we present the first all-optical time-resolved measurements of carrier dynamics in free standing semiconductor nanowires. Optical pump-probe measurements on GaN NW reveal a rapid transfer (<500 fs) of photoexcited carriers into states responsible for deleterious yellow luminescence, which can be modified by varying the growth and annealing temperatures. Polarization, angle, and wavelength-resolved measurements on vertically aligned Ge NW allow us to independently measure electron and hole dynamics parallel and perpendicular to the NW axis. Carriers propagating parallel to the NW axis have significantly longer lifetimes, clearly demonstrating the influence of two dimensional confinement on carrier dynamics in semiconductor nanowires.

8:48AM H24.00005 Optical Switching of Porphyrin-Coated Silicon Nanowire Field Effect Transistors, VINCENT BOUCHIAT, Neel Institute, CNRS-Grenoble, CLEMENS WINKELMANN, CNRS-Grenoble, IRINA IONICA, IMEP-MINATEC, XAVIER CHEVALIER, CHRISTOPHE BUCHER, GUY ROYAL, LEOPR — We study [1] porphyrin coated silicon nanowire field effect transistors, which display a large, molecule-dependent photoconversion process from the charge-to-current transducing effect of the semiconducting channel. The spectral dependence of the illumination wavelength and temperature. The decay kinetics from the high- to the low-conductance state is governed by charge recombination via tunneling, with a rate depending on the state of the SINW-FET. The comparison to porphyrin sensitized Carbon Nanotube FETs allows to distinguish the environment- and molecule-dependent photocurrent conversion process from the charge-to-current transducing effect of the semiconducting channel. The spectral dependence of the photoconductance agree with the UV-visible absorption spectrum of the isolated molecule [1]. Winkelmann et al, Nano Lett., vol. 7, p. 1454 (2007).

9:00AM H24.00006 Spectral dependence of thermal radiation from metallic nanowires on wire geometry, YAT-YIN AU, HELGI SKULI SKULASON, SNORRI INGVARSSON, Science Institute, University of Iceland, Dunhaga 3, Reykjavik IS-107, Iceland — We have studied the polarized Rayleigh back-scattering from individual silver nanowires. The nanowires were prepared by aqueous solution method and characterized by TEM lattice images and selected area diffraction (SAD) patterns. We found enhanced LO and TO phonon scattering near the tip of the nanowires. Spectra taken by Fourier Transform Infrared Spectrometry reveal strong suppression of radiation polarized perpendicular to the heater long axis as the heater width shrinks, while at the same time radiation polarized along the long axis of the heater approaches a constant value, resulting in highly polarized emission for heaters with very narrow width. We also observe a 2/θ-like resonance that we believe is associated with surface plasmon oscillations across the heater width. These findings have important implications for nanoscale thermal light generation.

9:12AM H24.00007 Anisotropic plasmon excitation and dispersion of Ag nanowires on Cu(110)1, T. SENEVIRATNE, ASOKA SEKHARAN, RICHARD KURTZ, PHILLIP SPRUNGER, Louisiana State University — Epitaxial Ag nanowires have been found to self-assemble on Cu(110) exceeding 1.2 ML. The plasmon excitation and dispersion of these nanowires have been characterized by low-energy reflection EELS. Previous STM images reveal that the Ag nanowires are approximately 2 nm (~12 nm) in height (width). However, the nanowires orientate with the long axis parallel to the [1 1 0] substrate direction and possess an anisotropic morphology. EELS reveals that the Ag plasmon excitation of 3.7 eV at the zone-center and is nearly dispersionless perpendicular to the nanowire direction. However, parallel to the Ag nanowires, EELS shows a slight red-shift of the plasmon at q = 0 and disperses to higher energy with increasing momentum transfer. These results will be discussed in light of recent ARPES band-structure measurements, electronic calculations, and anisotropic optical measurements of the Ag nanowires.

1Supported by NSF/DMR-050465

9:24AM H24.00008 Enhanced Raman Scattering Near the Tip of Semiconducting Nanowires, QIUJIE LU, JIAN WU, AWNISH GUPTA, Department of Physics, Penn State University, PETER EKLUND, Department of Physics, Department of Materials Science and Engineering, Penn State University — Results of polarized microRaman scattering experiments are presented on individual ~20μm long crystalline GaP nanowires (NWs) using 514.5 nm excitation. The NWs were supported on Transmission Electron Microscope (TEM) grids. The diameters of the NWs were characterized by TEM lattice images and selected area diffraction (SAD) patterns. We found enhanced LO and TO phonon scattering near the tip of the nanowire, i.e., the scattering is at least a factor of 5x stronger at the tip than observed at distances many microns away from the tip. The polarized scattering patterns I(θ), where θ is the angle between the incident electric field and the NW axis, also change as the probe beam approached the tip of the nanowires. The effects observed here should be general and apply to other semiconducting nanowire systems as well.

9:36AM H24.00009 Polarized Rayleigh Back Scattering from Individual GaP Nanowires, JIAN WU, G. CHEN, QIUJIE LU, P.C. EKLUND — Results of polarized Rayleigh back-scattering studies are reported for individual ~20 μm long crystalline GaP Nanowires (NWs) using 514.5 nm excitation. The NWs were determined by TEM. Positions of characteristic LO, TO phonon Raman bands were found to agree with bulk GaP. The Rayleigh back-scattering intensity polar pattern I(θ) was measured at room temperature, where θ is the angle between the incident electric field and the NW axis. The scattered radiation was polarized parallel to the incident electric field. For small NW diameter (d~70) nm, we observed ~ cos^4[θ] polar patterns. With increasing NW diameter above 100 nm, the polar scattering patterns rotate by 90° with respect to those seen in small diameter NWs and then they broaden to a circle. Our experimental data will be compared to the calculated Rayleigh back-scattering efficiency calculated via the Discrete Dipole Approximation (DDA). Our DDA calculations show that the polar patterns are sensitive to both the diameter and the NW length. Although the calculated polar patterns qualitatively support our data, improvement in the modeling is still needed. This work is supported by NSF NIRT, grant DMR-0304178.
10:00AM H24.00011 Optical Antenna Effect in Semiconducting Nanowires, P.C. EKLUND, JIAN WU, G. CHEN, QIUI JIE LIU, H.R. GUTIERREZ, QIHUA XIONG, M.E. PELLEN, J.S. PETKO, D. WERNER — Using Raman scattering, we have observed strong optical antenna effects which we identify with internal standing wave photon modes of the wire. The antenna effects were probed in individual GaP NWs whose diameters are in the range 40<\text{d}<300 \text{ nm}. The data and our calculations show that the nature of the backscattered light is critically dependent on the interplay between a photon confinement effect and bulk Raman scattering. At small diameter, d<65 \text{ nm}, the NWs are found to act like a nearly perfect dipole antenna and the bulk Raman selection rules are masked leading to a polarized scattering intensity function I(\theta) \sim \cos^2 \theta. For larger wires, many other different polar patterns are found. Underscoring the importance of this work is the realization that a fundamental understanding of the “optical antenna effect” in semiconducting NWs is essential to the analysis of all electro-optic effects in small diameter filaments.

10:12AM H24.00012 Spatially-Resolved Photoluminescence Mapping of Single CdS Nanosheets1, M. FICKENSHIER, T.B. HOANG, L.V. TITTOVA, A. MISHRA, L.M. SMITH, H.E. JACKSON, University of Cincinnati, J.M. YARRISON-RICE, Miami University, H. RHÖ, K.-Y. LEE, Chonbuk National University, Y.-J. CHOI, K.J. CHOI, J.-G. PARK, KIST — We present results of spatially-resolved low temperature photoluminescence of single 5 micron wide CdS nanosheets. The sheets, grown by pulsed laser deposition using vapor-phase transport, are uniform in size and shape and exhibit a hexagonal wurtzite structure. The orientation of the c-axis determined by PL polarization analysis and HR TEM varies from sheet to sheet. The spatially-resolved PL reveals spectral variation across the sheet, with A-like excitons at the edges showing a spectral peak at 2.54eV, and B-like excitons at the center showing a peak at 2.563eV. Exciton lifetimes of \sim 200 ps are observed, which are significantly longer than CdS nanowires of identical diameter, but shorter than measured in bulk CdS.

1Support provided by NSF (\#0701703), Korea Research Foundation and KIST.

10:24AM H24.00013 Anomalous Photoluminescence in CdSe Quantum Dot Solids at High Pressure due to Non-uniform Stress, S. SEBASTIEN HAMEL, C. CHRISTIAN GRANT, J. JONATHAN CROWHURST, A. ANDREW GUPTA, JIAN WU, P.C. EKLUND — Results of polarized micro-Raman scattering from LO and TO phonons in individual GaP nanowires (NWs) with different diameter and length are reported. The NW diameters were determined by Atomic Force Microscope (AFM) and length was measured by Scanning Electron Microscope (SEM). NWs with the same growth direction but variable length were prepared by cutting \sim 40 \mu m long wires into segments using a Focused Ion Beam. The polar plots of the back scattered intensity I_{\text{TO,LO}}(\theta) from these segments were collected, where \theta is the angle between the incident electric field and the NW axis. Interestingly, the shapes of these polar patterns depend on both the length and diameter of the NWs. The Raman scattering intensities for short wires (i.e., L<<1\mu m) also exhibit a non-linear dependence on the incident laser power I_0. The non-linearity increases with decreasing NW length and behaves as \sim I_0^4, for the shortest wires measured so far (i.e., L\sim 500 \mu m). Our results strongly suggest strong enhancement in the internal electric field via antenna effects. This work is supported by NSF NIRT, grant DMR-0304178.

10:36AM H24.00014 Dynamics of Photo-Excited Carriers in Single InP Nanowires Under High Excitation Density1, L.V. TITTOVA, T.B. HOANG, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, Y. KIM, H.J. JOYCE, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — The dynamics of photo-excited carriers in single InP nanowires at low temperature is investigated using time-resolved photoluminescence spectroscopy. Under highly intensity excitation, the photoluminescence spectrum from a single nanowire shows a broad emission band at early times after the excitation pulse indicating the presence of a degenerate, high density electron-hole plasma. At later times (> 600 ps) when the density of carriers decreases, the emission spectrum becomes narrower and converges toward the free exciton emission band. The lifetime of free excitons in a single nanowire is measured to be close to the lifetime of excitons in high quality InP epilayers, indicating the relative insensitivity of the carriers to the InP nanowire surface. These results indicate that significant state filling and band gap renormalization occur in single InP nanowires.

1Support for this work was provided by NSF (\#0701703) and the Australian Research Council.

10:48AM H24.00015 Near Infrared Photoresponse in Annealed CdSe Nanocrystal Films, LIWEI LIU, PAUL STOKES, ARTEM E. MASUNOV, SAIFUL I. KHONDAKER, NANOSCIENCE TECHNOLOGY CENTER, DEPARTMENTS OF PHYSICS & CHEMISTRY, UNIVERSITY OF CENTRAL FLORIDA TEAM — We found unexpected near infrared (NIR) photoresponse in CdSe nanocrystal superlattice film annealed above 400 C in air. The current voltage characteristic measured in a planar device geometry show a large increase in NIR current over dark current. The calculated external quantum efficiency of the device is up to 10.6 % at -5V and the responsivity is 0.7A/W obtained under 1.32 \mu W IR irradiation. UV-VIS absorption of annealed CdSe shows the redshifting and broadening of exciton peak and a decrease of band gap as the annealing temperature is increased. TEM image show that CdSe nanocrystals have been melted to fuse to different size distribution nanoparticles during annealing. We discuss possible reason for this unexpected behavior.

Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H25 DPOLY: Adsortion of Organics on Surfaces Morial Convention Center 217

8:00AM H25.00001 Polymer Physics Prize Break –
8:36AM H25.00002 Examining the air-water interfacial activity of beta-peptides using molecular simulation and experiment. CLARK A. MILLER, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — Amphiphilic beta-peptides (oligomers of beta-amino acids) are predicted to adsorb at the air-water interface using computer simulation and verified using experiments. Molecular dynamics simulations are used to calculate the free energy of adsorption for different degrees of amphiphilicity and different display of hydrophilic groups. Adsorption of selected peptides is examined by measuring the surface tension of a solution of beta-peptides at different concentrations and agreement with simulation results is found. Simulations show that 2/3 hydrophobic residues lead to favorable adsorption at the air-water interface while 1/3 hydrophobic residues is unfavorable. We analyze changes in the conformational properties and angle with the interface to understand the manner of adsorption. We further investigate the behavior of multiple peptides at the interface using computer simulation and determine the surface pressure and peptide-peptide interactions at the interface.

8:48AM H25.00003 Why are hyperactive ice-binding-proteins so active? IDO BRASLAVSKY, YELIZ CELIK, NATALYA PERTAYA, YOUNG EUN CHOI, Physics Department, Ohio University, Athens, OH, MAYA BAR, Structural Biology, Weizmann Institute of Science, Rehovot, Israel, PETER L. DAVIES, Department of Biochemistry, Queen’s University, Kingston, Ontario, Canada — Ice binding proteins (IBPs), also called ‘antifreeze proteins’ or ‘ice structuring proteins’, are a class of proteins that protect organisms from freezing injury. These proteins have many applications in medicine and agriculture, and as a platform for future biotechnology applications. One of the interesting questions in this field focuses on the hyperactivity of some IBPs. Ice binding proteins can be classified in two groups: moderate ones that can depress the freezing point up to ~1°C and hyperactive ones that can depress the freezing point several-fold further even at lower concentrations. It has been suggested that the hyperactivity of IBPs stem from the fact that they block growth out of specific ice surfaces, more specifically the basal planes of ice. Here we show experimental results based on fluorescence microscopy, highlighting the differences between moderate IBPs and hyperactive IBPs. These include direct evidence for basal plane affinity of hyperactive IBPs, the effects of IBPs on growth-melt behavior of ice and the dynamics of their interaction with ice.

1Support: BNNT and NQPI at Ohio University & CIHR to PLD.

9:00AM H25.00004 Probing (bio)-organic monolayers at the metal/air and metal/liquid interface by sum-frequency generation spectroscopy, FRANCESCA CECCHET, DAN LIS, YVES CAUDANO, CHRISTOPHE SILIEN, ALAA ADIN MANI, PAUL THIRY, ANDRÉ PEREMANS, LLS Laboratory of Lasers of Spectroscopies, FUNDP - University of Namur — In the present work, ordered monolayers of thios prepared by self-assembly (SAM), and of lipids obtained by the Langmuir-Blodgett technique (LB), have been studied by sum frequency generation spectroscopy (SFG) at the metal/air and metal/liquid interface, in different sets of polarizations. This study is focused on the determination of the molecular orientation (i.e. the tilt angle and the twist angle of the axis and of the plane of the molecular groups, respectively) and on the analysis of the interactions occurring within the layers or with outer target molecules.

9:12AM H25.00005 Flow Induced Growth of Striped Alkane Monolayers, M. BAI, H. TAUB, A. DIAMA, U. Mo.-Columbia, K. KNORR, U. des Saarlandes, U. G. VOLKMANN, P. U. Catolica Chile, F. Y. HANSEN, Tech. U. of Denmark — We report our observation of the growth of striped monolayer phases of alkanes when deposited from a solution under flow. AFM measurements show that the structure and morphology of dotriacontane (n-C32H66 or C32) films grown from solution depend sensitively on the flow direction over a SiO2-coated Si(100) substrate. The C32 film exhibits one or two layers adjacent to the SiO2 surface in which the molecules are oriented with their long axis parallel to the interface followed by a striped monolayer of perpendicularly oriented molecules. The stripes form along the direction of solution flow with typical dimensions of a few micrometers wide and a few hundred micrometers long, depending on the solution concentration. A striped morphology is also observed for C29 grown under similar conditions. Grazing incident-angle x-ray diffraction measurements indicate that the C32 stripes are crystalline and can be indexed by a rectangular unit cell. We offer some speculations on the origin of the striped morphology.

1Supported by Grant Nos. NSF DMR-0411748 and DMR-0705974 and FONDECYT 1060628 and 7070248.

9:24AM H25.00006 Molecular dynamics studies of the structure and dynamics of “perpendicular” layers of n-alkane molecules adsorbed on a solid substrate, F.Y. HANSEN, Tech. Univ.of Denmark, P. SOZA, P.U. Catolica Chile, H. TAUB, U.Mo.-Columbia, U.G. VOLKMANN, P.U. Catolica Chile — Both AFM and ellipsometry studies of n-alkane films adsorbed on a solid substrate from a solution have shown wetting and de-layering phenomena. It was found that on top of one or two “parallel” layers of molecules, where the long axis of the molecules is parallel to the surface, “perpendicular” layers of molecules are formed with the long axis of the molecules perpendicular to the surface. MD simulations of layers of tetracosane, n-C32H66, molecules are set up to answer the following questions about the “perpendicular” layers: a) Is the melting transition driven by gauche defect creations in the alkane chains like in the parallel layers?, b) can a rotator phase be identified?, c) is there a lateral translational mobility of the chains prior to melting?, and d) what is the mechanism driving the wetting and de-layering transitions in the films? 2H. Mo et al. Chem. Phys. Lett. 377, 99 (2003)

1Supported by Grant Nos. U.S. NSF DMR-0705974, FONDECYT 1060628, CONICYT, and the Danish Center for Scientific Computing .

9:36AM H25.00007 Structure and Phase Transitions of Vapor-Deposited C32 Films, V. DEL CAMPO, E.A. CISTERNAS, I. VERGARA, T. CORRALES, U.G. VOLKMANN, P.U. Catolica Chile, M. BAI, S.-K. WANG, H. TAUB, U.Mo.-Columbia, H. MO, S.N. EHRLICH, Brookhaven Nat. Lab — We have compared the structure, topography, and phase transitions of dotriacontane films (n-C32H66 or C32) that have been vapor-deposited onto a SiO2-coated Si(100) wafer with those that have been deposited from solution. X-ray reflectivity measurements indicate that the as-deposited films differ in their morphology but share the following structural features at room temperature: adjacent to the substrate there is a nearly complete bilayer in which the molecules are oriented with their long axis parallel to the surface. Above the parallel film are partial layers of molecules oriented perpendicular to the surface. After a heating cycle above the bulk C32 melting point (Tm), AFM images of all films show the presence of 3D mesa-shaped bulk particles. On a second heating, AFM reveals the same succession of phase transitions for both film types in which a perpendicular monolayer spreads outward from the mesa-shaped particles below Tm, followed by a delaying transition to a 3D fluid droplets just above Tm. 2M. Bai et al., Europhys. Lett. 79, 26003 (2007).

1Supported by Grant Nos. NSF DMR-0705974 and FONDECYT 1060628 and 7070248.
9:48AM H25.00008 Thermodynamic Studies of n-Octane Thin Films Adsorbed on Magnesium Oxide(100), DAVID FERNANDEZ-CANOJTO, J.Z. LARESE, Oak Ridge National Laboratory — Thermodynamic properties of n-octane adsorbed on the MgO(100) surface were investigated using high-resolution adsorption isotherms in the temperature range of 225 K to 295 K. Two distinct adsorption steps were observed in all isotherms. The average area occupied by an n-octane molecule was estimated to be 139.1 Å². The temperature variation of the two dimensional compressibility was used to identify phase transitions near 265.9 K and 271.4 K for the first and second layers, respectively. COMPASS force field has been used to calculate the minimum energy configuration of a single n-octane molecule sited on the MgO (100) facet. Calculations suggest that the most likely configuration for the adsorbed molecule is with the carbon backbone parallel to the (100) plane, and with the center of mass atop the Mg²⁺ site. U.S. DOE, Materials Science Division under contract No. DE-AC05-00OR22725 operated by UT-Battelle, LLC, and the NSF under grant DMR-0412231.

10:00AM H25.00009 X-ray Atomic-Scale Analysis of Self-Assembled Monolayer Growth on Silicon, J.C. LIN, J. KELLAR, J. KIM, N. YODER, K. BEVAN, S. DATT, S. NGUYEN, M. HERSAM, M. BEDZYK — Organic functionalization of silicon is of interest for applications ranging from biosensing to molecular electronics. The efficiency of molecular devices heavily depends on the ordering of the structure. Traditionally spectroscopy is used to characterize bonding, but often the overall structure can be ambiguous. Our strategy is to combine a compliment of techniques, including AFM, XPS, XRR(X-ray reflectivity), XSW(X-ray standing wave), XRF(X-ray fluorescence), and DFT(Density functional theory) to determine the molecular configuration and packing density of Self-Assembled Monolayers (SAMs) grown on H-passivated Silicon. Our periodic DFT study of 4-bromo-phenyl-acetylene (BPA) predicts that the local packing density can affect the Br height by as much as 2 angstrom. XSW, which is used to measure the 3D Br distribution shows that the local structure is unchanged when the average SAM coverage is increased. This indicates the type of 2D island nucleation growth process being observed. Comparison between 4-bromostyrene (BrSty) and BPA SAMs provides direct evidence that the double bond root of the BPA contributes to a stiffer configuration than the single bond root. With the aromatic rings in the structure for conducting electrons, BrSty and BPA molecules are a starting point for future molecular electronic designs with more complex molecules.

10:12AM H25.00010 ABSTRACT WITHDRAWN

10:24AM H25.00011 STM/S of Polydiacetylene Nanowires on Gold and Graphite, LILI WANG, RAJIV GIRDHARAGOPAL, KEVIN KELLY, Rice University — The structural and electronic properties of 10,12-pentacosadiynoic acid (PCDA) monolayer films and polydiacetylene (PDA) nanowires on Au islands on a HOPG substrate have been studied using STM. Our results indicate that PCDA monolayer films can be formed on both HOPG and 1-2 monolayer (ML) Au islands, but arrange in small domains due to the dense Au clusters. The arrangement of PDA nanowires exhibits different collapse density, length and bending between Au and HOPG areas due to differing chemical and electronic interactions, which play an important role in the charge transfer between conducting polymers and electrodes in commercial devices. STM-tip induced nanowire cutting, desorption and polymerization is also observed, with the surrounding PCDA molecules restoring the packing nearly instantaneously. This implies that the interaction with Au clusters is not strong enough to weaken the intramolecular interactions that produce the reordering cascade effect, although it strongly influences the arrangement of the nanowires. Furthermore, the local work function and dI/dV images indicate electronic structure differences between PCDA monolayer films on 1 ML Au islands and those on 2 ML islands, and between PDA nanowires on HOPG and those across Au islands.

10:36AM H25.00012 Thermodynamic and Neutron Scattering Investigation of Ethylene Wetting on MgO (100), ANDI BARBOUR, University of Tennessee, CRAIG BROWN, NIST Center for Neutron Research, J. Z. LARESE, Oak Ridge National Laboratory and University of Tennessee — The adsorption properties of a molecular film on a solid substrate are governed by the relative strength of the molecule-substrate versus molecule-molecule interaction. The wetting properties of ethylene (C₂H₄) molecular thin films on graphite are of fundamental interest because the number of observed adlayers increases as the intermolecular temperature increases with T<104K (bulk triple point). In adsorbate/substrate systems like C₂H₄/graphite, it is accepted that triple point wetting occurs. For our studies, we employed MgO nanocubes because they represent a prototypical metal oxide with a wide variety of technological uses including catalyst support. Of particular interest are wetting/layering transitions and the changes that take place in the neighborhood of the bulk triple point. We report our experimental investigation of the adsorption behavior of evidence C₂H₄ on MgO (100) using high-resolution adsorption isotherms and neutron diffraction and scattering. We demonstrate the dominance role that molecule-molecule interaction plays in the wetting phenomena by comparing the behavior of ethylene on graphite and MgO. U.S. Department of Energy (DE-AC05-00OR22725) at ORNL managed and operated by UT-Battelle, LLC, and the NSF (DMR-0412231).

10:48AM H25.00013 Importance of Van Der Waals Interaction for Organic Molecule-Metal Junctions, PRIYA SONNY, PETER PUSCHNIG, DMITRI NABOK, CLAUDIA AMBROSCH-DRAXL, Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Strasse 18, A–8700 Leoben, Austria — We present calculations to study the interface energetics of a weakly adsorbed organic molecule on metallic surfaces, which serve as model interfaces relevant for organic electronics. Thereby we focus on the role of the exchange-correlation potential and, in particular, the van der Waals interaction. To this extent the thiophene molecule is relaxed on clean Cu(110) and Cu(110)-(2x1)O, and the adsorption energy corresponding to various positions and orientations of the molecule is calculated on the search for the most favorable adsorption site. The molecule is found to be more strongly bound on the clean Cu(110) surface with an adsorption energy of −0.50 eV, as compared to −0.30 eV on Cu(110)-(2x1)O. Nonlocal correlations, i.e., the van der Waals interaction is found to be solely reponsible for the binding in such weakly bound systems, while the commonly used generalized gradient approximations not only underestimate the adsorption energy but also provide the wrong physical picture for the binding. The adsorption of thiophene lowers the work function of the metallic substrate due to the formation of surface dipoles while no sizeable charge transfer is found.

Tuesday, March 11, 2008 8:00AM - 11:00AM
Session H26 DCP; Focus Session: Photophysics of Cold Molecules IV, Morial Convention Center 218

8:00AM H26.00001 Reactions of cold trapped anions, ROLAND WESTER, Physikalisches Institut, Albert-Ludwigs-Universitaet Freiburg, Herrmann-Herder-Str. 3, 79104 Freiburg, Germany — Interactions of negative ions with small organic molecules represent model systems for the investigation of reaction dynamics in few-body systems. Their corrugated potential energy landscape, originating in long-range attractive and short-range repulsive forces, requires the coupling of different degrees of freedom for reactions to occur. We have adopted two complementary approaches to study anion-molecule reaction dynamics. Using velocity map imaging in combination with crossed beams at low energy we study the differential cross section of negative ion reactions. For nucleophilic substitution reactions we have observed several distinct reaction mechanisms when varying the collision energy [1]. Total reaction rate measurements, which we carry out in the box-shaped potential of a 22pole ion trap [2], have revealed unexpected temperature-dependences for proton transfer and for cluster stabilisation at low temperatures. In addition, laser-induced photodetachment is studied in the trap to obtain absolute destruction cross sections for negative ions in light fields [3]. These results are relevant for the understanding of the negative ion abundances in interstellar molecular clouds.

8:36AM H26.00002 Cold reactive collisions between laser-cooled ions and velocity-selected neutral molecules, MARTIN BELL, STEFAN WILLITSCH, ALEXANDER GINGELL, SIMON PROCTOR, TIMOTHY SOFTLEY, Department of Chemistry, University of Oxford — The recent development of a range of techniques for producing cold molecules at very low translational temperatures T < 1 K in the gas phase has provided the opportunity for studying molecular collisions in a new physical regime. We report a new experimental method to study reactive collisions between ions and neutral molecules at very low temperatures which allows for tunable collision energies and a variety of chemically diverse reaction partners. Our technique relies on the combination of a quadrupole-guide velocity selector for the generation of cold polar molecules with a facility to provide strong electric fields at low velocities to control the trajectories of the ions. We present results from the collisions of cold OH atoms with He atoms with the goal of creating molecular complexes of low rotational and vibrational energy. From the quadrupole-guide, the strong localization and long trapping times of the ions allows chemical reactions to be studied at the single-particle level. In a proof-of-principle experiment, we have studied the chemical reaction between translationally cold CH$_2$F molecules and laser-cooled Ca$^+$ ions in a collision energy range corresponding to 1-10 K. The characteristics of our cold-molecule sources and the performance of the new technique as well as perspectives for further developments will be discussed.

8:48AM H26.00003 Demonstration of a three-dimensional trap for state-selected Rydberg atoms, STEPHEN HOGAN, FREDERIC MERK, ETH Zurich, Switzerland — Recent progress in the development of methods by which to decelerate and manipulate the translational motion of Rydberg atoms and molecules in the gas phase using static and time-varying inhomogeneous electric fields has led to the experimental realization of Rydberg atom optics elements including a lens, a mirror and a two-dimensional trap. These experiments exploit the very large electric dipole moments associated with Rydberg Stark states, and have demonstrated the possibility to stop a seeded, pulsed, supersonic beam of atomic hydrogen traveling with an initial velocity of 700 ms$^{-1}$ within 3 mm and 5 µs using electric fields of only a few kVcm$^{-1}$. With the goal of achieving complete control of a cloud of Rydberg atoms or molecules in three-dimensions, we have recently designed and constructed a three-dimensional electrostatic trap for these particles. The design of this trap will be presented along with the results of a series of experiments in which we have used the trap to confine, in three dimensions, a cloud of atomic hydrogen Rydberg atoms in states with principal quantum numbers around n = 50. The dynamics of the Rydberg atoms in the trap have been investigated by pulse field ionization and imaging techniques. Under favorable conditions, trapping times on the order of 150 µs have been observed, corresponding to the radiative lifetimes of the excited states.

9:00AM H26.00004 Measuring the role of alignment in a molecule optical lens, SIMON M. PURCELL, PETER F. BARKER, University College London — Far off-resonant pulsed lasers have been used to deflect and focus molecules via the molecular dipole force, which is proportional the effective polarisability of the species [1]. Molecules have an anisotropic polarisability, which in the presence of an intense linearly polarised optical field (10$^{12}$ Wcm$^{-2}$) causes the molecule to align with the field polarisation vector. This alignment occurs due to the creation of paddles states, which are superpositions of field free rovibronic states of the molecule [2]. alignment of the molecule with the electric field can result in a higher effective polarisability leading to an increased dipole force that can be used to tailor the properties of molecular optical elements. Using this property, we are studying how the field polarisation can be used to modify the focal length of the molecule optical lens, created by a focused laser beam. We will present calculations of this process and a comparison with our experiments on cold (3 K) carbon disulphide molecules focused by a Nd:YAG laser beam. [1] H.S Chung, B.S Zhao, S.H. Lee et al., J. Chem. Phys 114, 8293 (2001) [2] B. Friedrich, D. Herschbach, J. Phys. Chem. 99, 15688 (1995)

9:12AM H26.00005 Cold and ultracold polar molecules, JUN YE, JILA, NIST and Univ. of Colorado — Study of ultracold molecules promises important benefits such as novel control of chemical reactions and molecular collisions, precision measurement of fundamental physical properties, and new methods for quantum information processing and quantum simulations. We undertake two approaches aimed to produce cold, polar molecular samples. In the first approach, we work directly with ground-state polar molecules such as hydroxyl radicals (OH) or formaldehyde molecules (H$_2$CO): After Stark deceleration through an inhomogeneously distributed electric field, OH molecules are loaded into a magnetic trap at a density $\sim 10^{13}$ cm$^{-3}$ and temperature of 50 mK. An important advantage of magnetically trapping OH molecules is the freedom in applying an external electric field without significantly affecting the trap dynamics. The open geometry of the trap will enable experimental studies of cold, dipolar collisions subject to an external electric field. We will report our latest progress towards this goal. In the second approach we explore the possibility of producing ultracold polar molecules via association of two different atoms from ultracold atom gas mixtures near quantum degeneracy. Specifically, an interspecies Feshbach resonance between bosonic 87Rb and fermionic 40K permits efficient creation of heteronuclear Feshbach molecules. Subsequent optical spectroscopy reveals promising paths to efficiently transfer populations from the weakly bound to more deeply bound states. Progress on the production of these ultracold fermionic polar molecules will be reported.

9:48AM H26.00006 Experimental demonstration of electrostatic surface guiding for cold polar molecules, YONG XIA, YALING YIN, JIANPING YIN, Key Laboratory of Optical and Magnetic Resonance Spectroscopy, Department of Physics,East China Normal University — We demonstrate an electrostatic surface guiding for cold polar molecules over a long distance of 44.5 cm on a substrate by using a hollow electrostatic field. Cold molecules are generated by two parallel charged wires and a grounded metal-plate. We measure the transverse spatial distribution of the guided supersonic D$_2$O (including CH$_3$Br) molecular beam and its longitudinal velocity one, and study the dependence of the relative guiding efficiency and the transverse temperature of the guided molecular beam on the guiding voltage, also perform Monte-Carlo simulations and theoretical studies for the molecular guiding process, and our guiding scheme has some potential applications in molecule optics, such as molecular-beam splitter, integrated molecular optics, etc.


10:00AM H26.00007 Rotational Spectra of Methane in Helium-4, ROBERT ZILLICH, Kepler University, Linz, BIRGITTA WHALEY, University of California, Berkeley — We extend correlated basis function (CBF) theory, in combination with diffusion Monte Carlo simulations, to spherical top molecules solvated in superfluid He$^4$ droplets. Similarly to our previous CBF work on linear molecules, the rotational excitations of a spherical top molecule are renormalized by a self energy which contains the 4He density modulation around the molecule as coupling. Due to the high symmetry of this density in the case of solvated spherical molecules the rotation-4He coupling turns out to be weak, and the corresponding reduction of the effective rotational constant is small. Therefore, unlike for linear molecules, for spherical top molecules the symmetry of the gas phase rotational spectrum is not preserved. Instead, for excitations of total angular momentum $J > 2$, we find that the self energy induces a splitting of the rotational energies. We present here the rotational spectra of solvated linear C$_2$H$_6$ and rotational spectra of solvated spherical CH$_4$ and CD$_4$. The spectra of Ar-H$_2$O and O$_2$-H$_2$O exhibited the splitting of the rotational lines, which is due to the anisotropy of their intermolecular potential. We have analyzed the observed splittings in the spectra to determine the intermolecular potentials of Ar-H$_2$O and O$_2$-H$_2$O in droplets. These results are compared with the corresponding potentials previously studied in both experimentally and theoretically.

10:12AM H26.00008 Water containing molecular complexes studied by superfluid helium droplet spectroscopy, SUSUMU KUMA, The University of British Columbia, MIKHAIL SLIPCHENKO, Iowa State University, TAKAMASA MOMOSE, The University of British Columbia, ANDREY VILESOV, University of Southern California — Superfluid helium droplets offer an ideal environment for spectroscopic studies of molecular complexes by virtue of the controllable aggregation process of embedded molecules and its weak interaction as a matrix medium. Here, we report the infrared spectroscopy of Ar-H$_2$O, N$_2$-H$_2$O, and O$_2$-H$_2$O complexes picked up in He droplets. The observed spectra in the anti-symmetric stretching vibrational region ($\nu_2$) of water around 3750 cm$^{-1}$ indicated that the water molecule in complexes rotates nearly freely in Ar-H$_2$O and O$_2$-H$_2$O, while not in N$_2$-H$_2$O. The spectra of Ar-H$_2$O and O$_2$-H$_2$O exhibited the splitting of the rotational lines, which is due to the anisotropy of their intermolecular potential. We have analyzed the observed splittings in the spectra to determine the intermolecular potentials of Ar-H$_2$O and O$_2$-H$_2$O in droplets. These results are compared with the corresponding potentials previously studied in both experimentally and theoretically.
10:24AM H26.00009 Microwave spectroscopy of doped helium clusters and doped helium droplets, WOLFGANG JÄGER. University of Alberta — High resolution microwave and infrared spectroscopy of small to medium sized doped helium clusters, e.g. He$_2$-OCS with $N$ from 2 to 70, has given detailed insights into how superfluidity, a bulk phase property, evolves from the microscopic scale. Some of the most significant findings were oscillatory behavior of cluster rotational constant $B$ with number of helium atoms, $N$, and the observation of very narrow lines (15 kHz in microwave and 0.001 cm$^{-1}$ in the infrared region), even for the largest $N$. How can this be reconciled with the broad (up to several GHz wide) lines of rotational and ro-vibrational transitions of molecular dopants in helium droplets? Microwave experiments of molecular dopants embedded in helium nanodroplets can help answer this question. We have measured the pure tunneling inversion transition of ammonia in helium droplets at about 20.7 GHz. A complex line shape, consisting of a sharp (15 MHz wide) line on top of a broad background (1.5 GHz wide) was observed. The line shape could be simulated by assuming identical energy sublevels of the initial and final state of the transition. This provides direct evidence for the existence of an energy level substructure of molecular states in doped helium droplets. Microwave rotational transitions of carbonylsulfide, OCS, in helium droplets show increase in line width with increasing rotational quantum number $J$ and, in some cases, prominent fine-structures. Some of these features can be interpreted in terms of droplet size distribution.

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H27 DCMP: Correlated Electrons: Heavy Fermions and Exotic Magnets

8:00AM H27.00001 Magnetism and metallicity in FeSb2-xTex, CEDOMIR PETROVIC, RONGWEI HU, Condensed Matter Physics, Brookhaven National Laboratory; VESNA MITROVIC, Physics Department, Brown University — Single crystals of FeSb2-xTex (0<x<1) were grown by molten metalin technique. A rich variety of electronic and magnetic ground states will be presented.

8:12AM H27.00002 Phase transitions in R$_5$NiPb$_3$ (R=Ce,Nd,Gd), V. GORUGANTI, K. D. D. RATHNAYAKA, JOSEPH H. ROSS, JR., Department of Physics, Texas A&M University — We report magnetic and thermodynamic measurements for recently-synthesized R$_5$NiPb$_3$ (R= Ce,Nd,Gd) (hexagonal Hf$_5$CuSn$_3$-type structure), as well as non-magnetic La-based analogs. High-temperature Curie-Weiss fits yield effective moments of 2.43, 3.70 and 9.3 $\mu_B$ for Ce$_5$NiPb$_3$, Nd$_5$NiPb$_3$ and Gd$_5$NiPb$_3$, respectively. These are close to the R$^{12}$$_{12}$ $\mu_B$ values, showing that Ni is nonmagnetic in all cases. For Ce$_5$NiPb$_3$, a peak seen in both the magnetization and specific heat at 48 K indicates an apparent ferromagnetic transition at that temperature, which is also confirmed by field dependent heat capacity and a positive Curie-Weiss temperature. Nd$_5$NiPb$_3$ exhibits two magnetic transitions, an antiferromagnetic transition at 42 K and an apparently weak ferromagnetic canting transition at 8 K. Ce$_5$NiPb$_3$ shows a kink in both the magnetization and specific heat at 68 K indicating a ferro- or ferrimagnetic transition at that temperature, which is also confirmed by a positive Curie-Weiss temperature. For this material, ZFC and FC measurements show irreversibility at transition temperature. For Ce and Nd samples $M$-$H$ curves show metamagnetism at low temperatures. We will compare the results with the non magnetic analog La$_5$NiPb$_3$.

8:24AM H27.00003 Universal heat transport in the heavy-fermion superconductor CeIn$_5$, HAMIDEH SHAKERIPOUR, M.A. TANATAR, Département de Physique, Université de Sherbrooke, Sherbrooke, Canada, P. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA, LOUIS TAILLEFER, Département de Physique, Université de Sherbrooke, Sherbrooke, Canada — In superconductors with nodes in the gap, zero-energy quasiparticles give rise to a residual linear term in the thermal conductivity at T=0. When the quasiparticle density of states is linear in energy, this term is universal, in the sense that it does not depend on impurity concentration. Such universal heat transport has been observed in cuprates and ruthenates but never in heavy-fermion superconductors. Here we show that heat transport in the heavy-fermion superconductor CeIn$_5$ is unchanged by the doping of La impurities. This universal transport confirms the presence of a line node in the gap [1].

1$^{1}$Work supported by Office of Basic Energy Sciences US Department of Energy

8:36AM H27.00004 Fermi Surface Investigation of Cd doped CeCoIn$_5$, CIGDEM CAPAN, University of California Irvine, LUIS BALICAS, YOUN JUNG JO, National High Magnetic Field Laboratory, ROY GOODRICH, Louisiana State University, ANDREA BIANCHI, Université de Montréal, JOHN DITUSA, Louisiana State University, ZACHARY FISK, University of California Irvine — CeCoIn$_5$ is a 2.3K superconductor member of the 115 family of heavy fermion compounds that have attracted much attention due to the competing magnetism and superconductivity. The superconductivity in CeCoIn$_5$ emerges from a metallic state that exhibits strong deviations from the Fermi Liquid theory, with the presence of a field-tuned antiferromagnetic quantum critical point near the upper critical field. Recently it was shown that Cd substitution can tune the ground state from superconducting to antiferromagnetic. One important question is how the shape of the Fermi surface influences the stability of the ground state. We will present de-Haas van-Alphen results in Cd doped LnCoIn$_5$ (Ln=La,Ce) and discuss the origin of magnetic order in this system.

8:48AM H27.00005 Two fluid analysis of La and Cd doped CeIn$_5$, NICHOLAS BERRY, University of California Irvine, ANDREA BIANCHI, Université de Montréal, ZACHARY FISK, University of California Irvine — The heavy fermion superconductor CeIn$_5$ has been shown to have a ground state dependence on Cd doping which induces antiferromagnetism while suppressing superconductivity. This system provides an interesting regime in which to study the whole range of the heavy fermion superconducting and antiferromagnetic ground states as well as the interplay between the different electronic interactions at low temperatures. The Two Fluid Model has quantified the energy scales in the related La doped CeCoIn$_5$. We attempted a two fluid analysis on specific heat and susceptibility measurements of La and Cd doped CeIn$_5$ single crystals.

9:00AM H27.00006 Anisotropic effect of Cd-doping on superconducting phase in CeIn$_5$ at high fields, YOSIFUMI TOWIKI, ROMAN MOVSHOVICH, FILIP RONNING, ERIC BAUER, Los Alamos National Laboratory, ANDREA BIANCHI, Département de Physique, Université de Montréal, Montreal, QC, H3C 3J7, Canada; LOS ALAMOS NATIONAL LABORATORY TEAM, DEPARTEMENT DE PHYSIQUE, UNIVERSITE DE MONTREAL, MONTREAL, QC, H3C 3J7, CANADA COLLABORATION — Unconventional superconductor CeCoIn$_5$, at high magnetic field displays first order superconducting (SC) transition, and an additional high field-low temperature SC phase (previously proposed to be an inhomogeneous superconducting FFLO state). We have studied Cd-doping effect on the FFLO state and the first order SC transition by measuring specific heat C(T) of CeCoIn$_{5-x}$Cd$_{x}$ (x=0.01, 0.02 and 0.03) at low temperatures and high fields. Our data show that the FFLO state is already destroyed by 1% Cd-doping. The effect of Cd doping on the first order SC transition is anisotropic. The cross-over temperature $T_{c}$, where the superconducting transition changes its nature from first to second order, decreases rapidly with increasing doping for $H/H_{c1}$ and disappears already at $x=0.02$, while it remains rather temperature-independent for $H/H_{c1}$ up to $x=0.03$. 

9:12AM H27.00007 Angular Dependent Magnetic Properties of CeCoIn$_5$ at Low Temperatures$^\ddagger$
J.-H. PARK, R.L. STILLWELL$^\ddagger$, T.P. MURPHY, E.C. PALM, S.W. TOZER, NHMFL, Florida State University, Tallahassee, FL 32310, J.C. COOLEY, LANL, MST-6, Los Alamos, NM 87545 — The heavy-fermion compound CeCoIn$_5$ exhibits a superconducting transition at 2.3 K. As an unconventional superconductor, many unusual physical properties of the compound have been actively studied. In particular, evidence of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting state in this compound was reported first by Radovan and co-workers. At the lowest temperature (20 mK), the FFLO state of CeCoIn$_5$ was observed in fields between 10 and 11.7 T when the ab-plane of the compound was placed parallel to the external magnetic field. In addition, at these low temperatures, the angular dependent peak effect was observed and interpreted as a crossover between Abrikosov and Josephson vortex lattices. Further experimental studies of the low temperature (> 20 mK) magnetic properties of CeCoIn$_5$, performed in various sample orientations with respect to magnetic field will be presented. H.A. Radovan, et al., Nature 425 (2003) 51. H.A. Radovan, et al., Philosophical Magazine 86 (2006) 3569.

9:24AM H27.00008 Evolution of the FFLO state of CeCo(In$_{1−x}$Hg$_x$)$_5$ by incommensurate antiferromagnetic order. SEIKO OHIRA-KAWAMURA, Ochanomizu Univ., HIROAKI SHISHIDO, Kyoto Univ., AKARI YOSHIDA, Ochanomizu Univ., RYUJI OKAZAKI, Kyoto Univ., HAZUKI KAWANO-FURUKAWA, Ochanomizu Univ., TAKASADA SHIBAUCHI, Kyoto Univ., HISATOMO HARIMA, Kobe Univ., YUJI MATSUDA, Kyoto Univ. — CeCoIn$_5$ shows superconductivity (SC) below 2.3 K, while the SC is highly suppressed in a related system CeRhIn$_5$, which exhibits the antiferromagnetic (AF) order below 3.8 K. Then the mixed compound CeRh$_{1−x}$CoIn$_5$ is expected to have a complex $x$-T phase diagram where the SC and magnetism coexist. In order to understand the relationship between the SC and the antiferromagnetism in CeRh$_{1−x}$CoIn$_5$, we have performed neutron diffraction measurements on this system for various $x$. A commensurate (C) AF order with a propagating vector $q_c = (1/2, 1/2, 1/2)$ simultaneously appears. We interpret that there is no intrinsic coexistence between the IC- and C-AF orders and that the SC competes with the IC-AF order but coexists with the C-AF one. These results imply that particular areas on the Fermi surface nested by $\vec{q}_c$ play an active role in forming the superconducting state in CeCoIn$_5$.

9:36AM H27.00009 Supression of superconductivity in CeRh$_{1−x}$CoIn$_5$ by incommensurate antiferromagnetic order. SEIKO OHIRA-KAWAMURA, Ochanomizu Univ., HIROAKI SHISHIDO, Kyoto Univ., AKARI YOSHIDA, Ochanomizu Univ., RYUJI OKAZAKI, Kyoto Univ., HAZUKI KAWANO-FURUKAWA, Ochanomizu Univ., TAKASADA SHIBAUCHI, Kyoto Univ., HISATOMO HARIMA, Kobe Univ., YUJI MATSUDA, Kyoto Univ. — CeCoIn$_5$ shows superconductivity (SC) below 2.3 K, while the SC is highly suppressed in a related system CeRhIn$_5$, which exhibits the antiferromagnetic (AF) order below 3.8 K. Then the mixed compound CeRh$_{1−x}$CoIn$_5$ is expected to have a complex $x$-T phase diagram where the SC and magnetism coexist. In order to understand the relationship between the SC and the antiferromagnetism in CeRh$_{1−x}$CoIn$_5$, we have performed neutron diffraction measurements on this system for various $x$. A commensurate (C) AF order with a propagating vector $q_c = (1/2, 1/2, 1/2)$ simultaneously appears. We interpret that there is no intrinsic coexistence between the IC- and C-AF orders and that the SC competes with the IC-AF order but coexists with the C-AF one. These results imply that particular areas on the Fermi surface nested by $\vec{q}_c$ play an active role in forming the superconducting state in CeCoIn$_5$.

9:48AM H27.00010 Chiral d-wave superconductivity in the heavy fermion compound CeIrIn$_5$. ADITYA RAGHAVAN, KAZUMI MAKI, STEPHAN HAAS, University of Southern California — A recent experiment by Shakeripour et al indicates that the superconductivity in heavy fermion compound CeIrIn$_5$ is very different from the one in CeCoIn$_5$. We have re-examined their data and concluded that it belongs to the chiral d-wave SC or $\Delta(k) \sim e^{i\pi k_x} \cos(k_z)$.

10:00AM H27.00011 Fabrication of artificial heavy fermion superlattices by the molecular beam epitaxy. HIROAKI SHISHIDO, TOMONARI KATO, MANABU IZAKI, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, TAKAKIOTO TERASHIMA, Research Center for Low Temperature and Materials Sciences, Kyoto University, Kyoto 611-0011, Japan — We have grown artificial superlattices of CeIn$_3$ ($m$) / LaIn$_3$ ($n$), in which $m$-layers of heavy-fermion antiferromagnet CeIn$_3$ and $n$-layers of a non-magnetic isostructural compound LaIn$_3$ are stacked alternately, by a molecular beam epitaxy. Growth process were monitored by reflection high energy electron diffraction (RHEED). Sharp streak pattern of RHEED indicates the epitaxial growth of thin films. Satellite peaks observed in a X-ray diffraction pattern also indicates the superlattice structure. By reducing the thickness of CeIn$_3$, we observe a suppression of antiferromagnetic order and an enhancement of effective mass inferred from the resistivity coefficient, which both imply new ‘dimensional tuning’ towards a quantum critical point.

10:12AM H27.00012 Antiferromagnetism in the Kondo lattice system Ce(Ni$_{0.25}$In$_{1−x}$)$_5$. W.H. LEE, H.H. WU, H.H. SONG, K.J. SYU, Department of Physics, National Chung Cheng University, Ming-Hsuing, Chia-Yi, Taiwan, ROC, Y.Y. CHEN, Academia Sinica, Nankang, Taipei, Taiwan, ROC, W.H. LEE/Y.Y. CHEN TEAM — The pseudobinary compound Ce(Ni$_{0.25}$In$_{1−x}$)$_5$, which crystallizes in a hexagonal AlB$_2$ type structure with space group P6/mmm, exhibits antiferromagnetic ordering below the temperature 3.9 K, as revealed in the magnetic susceptibility, electrical resistivity and low-temperature specific-heat data. A ln(T) dependence is seen in the high temperature region for the magnetic contribution to the resistivity $\rho_{mn}$, which is one of the characteristic features of dense Kondo systems. The magnetic entropy $S_m(T,N)$ associated with the magnetic structure of Ce(Ni$_{0.25}$In$_{1−x}$)$_5$ is found to be only 62% of Rin(2), corresponding to a reduction of 38% of the cerium moment. This large magnetic reduction may be able to be attributed to Kondo effect. The heat capacity C(T) of Ce(Ni$_{0.25}$In$_{1−x}$)$_5$ in the paramagnetic state at temperatures between 8 and 20 K, can be fitted to the expression $C_m = \gamma T + \beta T^3$ by a least squares analysis, which yields the value $\gamma = 123 mJ/mol K^2$ and $\beta = 1.2 mJ/mol K^4$, the latter value corresponding to the Debye temperature $\Theta_D = 169 K$.

10:24AM H27.00013 Angle dependent quasiparticle weights in correlated metals. POUYAN GHAEMI, Massachusetts Institute of technology, SENTHIL TODADIRI, Massachusetts Institute of Technology, PIERS COLEMAN, Rutgers University — The variation in the quasiparticle weight $Z$ on moving around the fermi surface in correlated metals is studied theoretically. Our primary example is a heavy Fermi liquid treated within the standard hybridization mean field theory. The most dramatic variation in the quasiparticle weight happens in situations where the hybridization vanishes along certain directions in momentum space. Such a “hybridization node” is demonstrated for a simplified model of a Cerium-based cubic heavy electron metal. We show that the quasiparticle weight varies from almost unity in some directions, to values approaching zero in others. This is accompanied by a similar variation in the quasiparticle effective mass. Some consequences of such hybridization nodes and the associated angle dependence are explored. Comparisons to somewhat similar phenomena in the normal metallic state of the cuprate materials are discussed. A phenomenological picture of the pseudogap state in the cuprates with a large Fermi surface with a severely anisotropic spectral weight is explored.
10:36AM H27.00014 Magnetic properties of RFe₂Zn₂₀ (R = Y, Gd - Lu): 4f moments embedded in strongly correlated electron host, SHUANG JIA, NI NI, A. SAFA-SEFAT, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory, USDOE and Department of Physics and Astronomy, Iowa State University, HYUNJIN KO, Ames Laboratory, USDOE and Department of Chemistry, Iowa State University — The RFe₂Zn₂₀ series of compounds manifest varied magnetic properties, from near ferromagnetism (R = Y, Lu), to enhanced ferromagnetic (FM) ordering of local moments (R = Gd to Tb), to heavy Fermi ground state (R = Tb). Thermodynamic and transport measurement results reveal that these varied magnetic states can be understood in the framework of 4f moments embedded in a nearly ferromagnetic Fermi liquid. In such a highly polarizable electronic host, the different type of 4f moments, null moments for Y³⁺ and Lu³⁺, pure spin- contributed Gd⁵⁺, spin-orbital-coupling contributed Tb⁵⁺ to Tb³⁺, and the hybridized Yb ions, correlated with the itinerant electrons, lead to this magnetic versatility. For local moment members (R = Gd to Tb), the Curie temperatures roughly scale with the de Gennes parameter, indicating negligible crystal electric field (CEF) effect on the magnetic ordering, although the CEF on the 4f local moments leads to anisotropic FM ground state for R = Tb to Tb. For hybridized moment member (R = Yb), the Kondo temperature seems to be enhanced, associated with the electronic host.

10:48AM H27.00015 Low-Energy Magnetic Excitations in the Itinerant Quantum Ferromagnet ZrZn₂, STEPHEN HAYDEN, EDWARD YELLAND, University of Bristol — High resolution de Haas-van Alphen measurements offer a powerful method to probe the low energy magnetic excitations in ferromagnets. Here we report measurements of the temperature dependence of the exchange splitting Δ(T) in the weak itinerant ferromagnet ZrZn₂ (Curie temperature Tc = 28 K) using the de Haas-van Alphen (dHvA) effect. Quantitative comparison with the magnetic moment M(T) shows that longitudinal or 'Stoner' excitations dominate, in strong contrast with observations on metallic ferromagnets like Fe and Ni, where spin-waves dominate at low T. We ascribe the difference to the proximity of a quantum critical point (QCP) in ZrZn₂. The results are discussed in terms of a phenomenological Ginzburg-Landau model which includes effects of thermal fluctuations and enhanced fluctuations due to the nearby quantum critical point. We find that the model accurately predicts both the rate of collapse of M(T) with T and the relative reduction of Δ(T) and M(T). We suggest a picture for the evolving nature of magnetic excitations within the ferromagnetic state as the QCP is approached.

Tuesday, March 11, 2008 8:00AM - 10:36AM –

Session H28 DCMP: Photonic Crystals Morial Convention Center 220

8:00AM H28.00001 Moving the band gaps and changing the transmission of magnetic photonic crystals, SHIYANG LIU, JUNJIE DU, ZHIFANG LIN, Fudan University, SIU TAT CHUI, University of Delaware — We classify different types of the photonic band gaps (PBGs) of two dimensional magnetic photonic crystals (MPCs) consisting of arrays of magnetic cylinders and study the different tunability (by an external static magnetic field) of these PBGs. One type of the band gaps comes from infinitely degenerate flat bands and is closely related to those in the study of plasmonics. We calculate the transmission of the PBG’s and found excellent agreement with the results of the photonic band structure calculation. Positional disorder of the lattice structure affects the different types of PBGs differently.

8:12AM H28.00002 Probing states with macroscopic circulations in magnetic photonic crystals, SIU TAT CHUI, University of Delaware, ZHIFANG LIN, Fudan University — We predict that when light is reflected off a magnetic photonic crystal (MPC) there is a grazing component that is parallel to the surface; the magnitude of this component can be changed by an external field. The direction of this parallel component is reversed (dotted line) as the direction of the magnetization is reversed. This provides a way to probe states with macroscopic circulations inside the MPC.

8:24AM H28.00003 Experimental investigation of photonic gaps in optical Thue-Morse multilayers fabricated using nanostructured thin films, MATTHEW HAWKEYE, University of Alberta, MICHAEL BRETT — One-dimensional Thue-Morse (TM) multilayers are realized by stacking together layers of different refractive index according to simple rules. The result is a deterministically generated aperiodic system representing an intermediate stage between a periodic medium and a random one. This work focuses on the formation of photonic gaps at musings frequencies relating to local positional correlations in the TM structure. TM multilayers are realized in the visible and near-IR spectral regions using glancing angle deposition (GLAD), a single-step nanofabrication technique providing control over the internal columnar structure of a deposited thin film. The effective refractive index of the deposited layer is tuned by controlling the columnar structure leading to great flexibility over the choice of refractive index in the experiment. Using GLAD, TM multilayers are fabricated out of titanium dioxide by varying the density of the columnar structures. The resulting photonic gaps are characterized using transmittance and reflectance spectroscopy and compared with the results of transfer matrix simulations. The creation of gaps in different generations of the TM system will also be examined.

8:36AM H28.00004 Effective medium theory of photonic crystals¹, W.T. LU, Department of Physics and Electronic Materials Research Institute, Northeastern University, Boston, MA 02115, S. ZHANG, Department of Mechanical Engineering, University of California at Berkeley, Berkeley, CA 94720, Y.J. HUANG, S. SRIDHAR, Department of Physics and Electronic Materials Research Institute, Northeastern University, Boston, MA 02115 — We develop an effective medium theory for photonic crystals including negative index metamaterials. This theory is based on field summation over the choice of refractive index in the experiment. Using GLAD, TM multilayers are fabricated out of titanium dioxide by varying the density of the columnar structures. The resulting photonic gaps are characterized using transmittance and reflectance spectroscopy and compared with the results of transfer matrix simulations. The creation of gaps in different generations of the TM system will also be examined.

¹This work was supported by the Air Force Research Laboratories, Hanscom (Contract # FA8718-06-C-0045) and the National Science Foundation (contract # PHY-0457002).

8:48AM H28.00005 Refraction at a photonic crystal surface: exact characterization¹, PRABASAJ PAUL, Denison University — Refraction at plane air-photonic crystal surfaces in a class of photonic crystals is studied. The class of photonic crystals has particularly simple band-structure and Bloch wave solutions, which make the evaluation of exact reflection and transmission coefficients relatively simple. New analytical results are presented, and the effects of variation in surface location and orientation are explored. A close look is taken at two important issues – negative refraction, and the validity of the Rayleigh hypothesis. The results obtained are consistent with those in existing literature.

¹Supported in part by the Research Corporation.
9:00AM H28.00006 Quantum interference near a photonic band edge beyond the weak field approximation. PAUL M. ALSING, DAVID A. CARDIMONA, DANHONG H. HUANG, Air Force Research Laboratory — We investigate spontaneous emission and quantum interference effects involving a three level atom in the vicinity of a photonic band edge, beyond the weak driving field approximation. We consider two different three-level atoms, each subject to a probe field from the ground state, and each embedded within a different photonic crystal (PhC). The first atom has the two excited states separated by a dipole transition in the optical frequency range, with this frequency being close to the surrounding PhC’s band edge. The probe field couples the ground state and the highest excited state, and is well outside the PhC bandgap. If a coupling field is applied between the two upper levels, Electromagnetically Induced Transparency (EIT) may occur, depending on the position of the band edge. The second atom has the two upper levels each dipole-coupled to the ground state, and close enough that the emissions from each can coherently interfere. This atom is embedded within a PhC whose band edge lies near the lower of the two excited states, and a probe field is applied that lies just beyond this band edge. This atom exhibits a quantum interference phenomenon related to EIT called Field-Induced Transparency (FIT), again depending on the position of the band edge relative to the lower excited state.

9:12AM H28.00007 Microwave transmission measurements through wire array photonic crystals. GRAEME DEWAR, University of North Dakota, NATHAN SOUTHER, MICHAEL JOHNSON — We have measured the microwave transmission between 12.4 and 18.0 GHz through wire arrays formed into two dimensional square lattices. One array made of copper wire 0.16 mm in radius consisted of five rows by 21 columns having a lattice constant of 5.15 mm. This array exhibited a pass band above 15 GHz, in good agreement with the calculated plasma frequency found from an expression for the permittivity derived in the long wavelength limit. A second array was made with wire of radius 18 microns and lattice constant 0.8 mm. This array was filled with dielectric loaded with powdered magnetite. A sample of this metamaterial 5.8 mm thick and with no externally applied magnetic field exhibited a pass band above 16 GHz. Implications for creating metamaterials with a negative index of refraction from wire arrays embedded in a magnetic host will be discussed.

9:24AM H28.00008 Tailoring Self-Assembled Metallic Photonic Crystals for Modified Thermal Emission. SANG EON HAN, Department of Chemical Engineering and Materials Science, University of Minnesota, ANDREAS STEIN, Department of Chemistry, University of Minnesota, DAVID NORRIS, Department of Chemical Engineering and Materials Science, University of Minnesota — Photonic crystals are solids that are periodically structured on an optical length scale. Previous work has shown that specific photonic crystal structures can lead to changes in the thermal emission spectra of a material. This may allow elimination of unwanted heat from emission sources, such as tungsten filaments in conventional light bulbs, or lead to new materials for thermophotovoltaics. Here, we study the possibility that metallic photonic crystals obtained via self-assembly can modify thermal emission. These structures, known as inverse opals, are easy to fabricate. However, experiments on tungsten inverse opals suggest that they also have strong optical absorption. In this case, the light does not interact sufficiently with the periodicity of the crystal and modification of thermal emission does not occur. We consider the origin of this effect and show theoretically how to tailor both absorption and surface coupling in experimentally realizable metallic inverse opals. Calculations for tailored inverse opals made from tungsten, molybdenum, and tantalum show that their optical properties can be similar to or even better than the tungsten woodpile structure, which has previously shown modified thermal emission.

9:36AM H28.00009 Integrated lenses for enhanced coupling into terahertz photonic crystal slab waveguides. CRISTO YEE, STEPHEN PARHAM, MARK SHERWIN, Physics Department and Institute for Quantum and Complex Dynamics, University of California Santa Barbara — The fundamental property of a photonic crystal (PC), its optical band gap, can be exploited by the introduction of defects that allow the existence of spatially localized states within the optical band gap. A PC waveguide consist of a line of defects in which the localized states will coalesce to form bands that allow the transmission of light otherwise prohibited. Coupling light directly from a source into the waveguide is restricted by the impedance mismatch of the PC waveguide and the surrounding media. In this work we use integrated lenses to enhance coupling of light into PC waveguides. PC slabs with lattices constants ranging from 56 to 64 microns were fabricated with Reactive Ion Etching on a high-resistivity Si wafer. An narrow band tunable source was employed to measure the transmission trough the waveguides. The results are compared with a full 3D FDTD calculations. This work was supported by NSF under grant CCF0507295 and CONACYT-UCMEXUS.

9:48AM H28.00010 Modeling Conformal Growth in Photonic Crystals and Comparing to Experiment. ANDREW BRZEZINSKI, YING-CHIEH CHEN, PIERRE WILTZIUS, PAUL BRAUN, Dept. of Mat. Sci. & Eng. / Beckman Institute / U. of Illinois, Urbana — Conformal growth, e.g. atomic layer deposition (ALD), of materials such as silicon and TiO$_2$ on three dimensional (3D) templates is important for making photonic crystals. However, reliable calculations of optical properties as a function of the conformal growth, such as the optical band structure, are hampered by difficulty in accurately assessing a deposited material’s spatial distribution. A widely used approximation ignores “pinch off” of precursor gas and assumes complete template infilling. Another approximation results in non-uniform growth velocity by employing iso-intensity surfaces of the 3D interference pattern used to create the template. We have developed an accurate model of conformal growth in arbitrary 3D periodic structures, allowing for arbitrary surface orientation. Results are compared with the above approximations and with experimentally fabricated photonic crystals. We use an SU8 polymer template created by 4-beam interference lithography, onto which various amounts of TiO$_2$ are grown by ALD. Characterization is performed by analysis of cross-sectional scanning electron micrographs and by solid angle resolved optical spectroscopy.

10:00AM H28.00011 The couple between modes of planar wave guides and the evanescent fields produced in the total internal reflection. RAUL GARCIA-LLAMAS, JORGE GASPAR-ARMENTA, Universidad de Sonora, RAMON MUNGUIA-ARVAYO, Posgrado en Fisica — The coupling between the modes of planar wave guides and the evanescent fields produced in the total internal reflection (TIR) system is studied theoretically. The planar guides are assumed as a semi-infinite inhomogeneous periodic medium (IM) with modulation only in the $y$-direction and period $a$, which is perpendicular to the propagation ($z$-axis) of the modes. This medium is separated by a vacuum (VA) gap, of uniform thickness $d_z$, from a semi-infinite homogeneous dielectric medium (HM). Then, two interfaces are found, one at $z = 0$ between HM/VA and other at $z = d_z$ between VA/IM. A transverse magnetic electromagnetic plane wave with wavelength $\lambda_0$, impinging the VA/IM interface and its wave vector, in the $z-\ y$ plane, is doing an angle $\theta_l$ with the $z$-axes. The solution of the electromagnetic diffracted field in the IM is a multimodal expansion as proposed by Burckhardt [J. Opt. Soc. Am. 56 (1966) pp. 1502]. Following the approach used by Glass and Maradudin [Phys. Rev. B 29 (1984) pp. 321] a matrix equation for the amplitudes of the diffracted field is found. Following the approach used by Glass and Maradudin [Phys. Rev. B 29 (1984) pp. 321] a matrix equation for the amplitudes of the diffracted field is found. Numerical solutions of the near field intensity are presented.

SEP-Conacyt 2004 PROYECTO C01-47391/A-1.
10:12AM H28.00012 Negative bi-refraction of acoustic waves in sonic crystals, YAN-FENG CHEN, Nanjing University, NATIONAL LABORATORY OF SOLID-STATE MICROSTRUCTURE COLLABORATION — Optical birefringence and dichroism are classical and important effects originating from two independent polarizations of optical waves in anisotropic crystals. However, it is impossible for acoustic waves in the fluid to show such a birefringence because only the longitudinal mode exists. The emergence of an artificial sonic crystal (SC) has significantly broadened the range of acoustic materials in nature that can give rise to acoustic bandgaps and be used to control the propagation of acoustic waves. Recently, negative refraction has gained a lot of attention and has been demonstrated in both left-handed materials and photonic crystals. Similar to left-handed materials and photonic crystals, negative refractions have also been found in SCs. Here we report the acoustic negative-birefringence phenomenon in a two-dimensional SC, even with the same frequency and the same “polarization” state. By means of this feature, double focusing images of a point source have been realized. This birefrigence concept may be extended to other periodic systems corresponding to other forms of waves, for example, electron for semiconductors, photon for photonic crystals, and plasmon for plasmonic crystals, showing great impacts on both fundamental physics and device applications.

10:24AM H28.00013 Random high-Q cavities in disordered photonic crystal waveguides, FRANK VOLLMER, JURAJ TOPOLANCÍK, Rowland Institute at Harvard — We demonstrate experimentally that structural perturbations imposed on highly dispersive photonic crystal-based waveguides give rise to spectral features that bear signatures of Anderson localization. Sharp resonances with effective Q’s of over 30,000 are found in scattering spectra of disordered waveguides. The resonances are observed in a ~20-nm bandwidth centered at the cutoff of slowly guided Bloch modes. The origin of the spectral features can be explained by the interference of coherently scattered electromagnetic waves which results in the formation of a narrow impurity (or localization) band populated with spectrally distinct quasistates. http://webmac[rowland.org]/rj/vollmer/index.php

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H29 DMP: Focus Session: Carbon Nanotubes and Related Materials VI: Graphene Transport Morial Convention Center 221

8:00AM H29.00001 Binary memory switching in zigzag-edge graphene nanostrips, DANIEL GUN-LYCKE, Naval Research Laboratory, DENIS A. ARESHKIN, George Washington University, JOHN W. MINTMIRE, JUNWEN LI, Oklahoma State University, CARTER T. WHITE, Naval Research Laboratory — Owing to a peculiar boundary condition, the ground state of any hydrogen-terminated zigzag-edge graphene nanostrip is predicted to exhibit spin-polarized edge states. We capture this physics in a model which has a Hamiltonian that consists of tight-binding terms and terms describing the potential from a spin-dependent scalar field. The model is solved in the presence of a ballistic current passing through the nanostrip. Studying the grand canonical potential for the system, it is shown that the spin-polarized state collapses above a certain bias. Below that threshold there is a bi-stable regime which could be exploited in a possible memory device. The memory could be both set and cleared through the bias and be read by measuring the current through the device.

8:12AM H29.00002 Graphene and Graphite Nanoribbons: phonon-scattering limit of conductivity from tight-binding, DANIEL FINKENSTADT, U.S. Naval Research Laboratory, GARY PENNINGTON, U.S. Army Research Laboratory, MICHAEL MEHL, U.S. Naval Research Laboratory — To understand nanoribbons of graphene, and multilayers of such ribbons, we developed an ab initio parametrized fit to Carbon and Hydrogen chemical data, out to arbitrary neighbor interactions, including relaxations [Phys. Rev. B 76, 121405R (2007)]. Our computed band structure shows a decrease in the armchair edge band gap when ribbons are multilayered. Further, the well-known three-family behavior of armchair bangaps is confirmed and shown here to apply also to the drift velocity of charge carriers, which can have ±20% deviation from the ideal Fermi velocity. Boltzmann carrier transport simulations from calculated phonon spectra also show a familiar dependence of conductance, peak field-effect mobility and “on” conductance that increase linearly with ribbon width. We will also discuss phonon-limited scattering of charge carriers in graphene multilayers and the temperature dependence of transport.

8:24AM H29.00003 Spin transport in rough graphene nanoribbons, INANÇ ADAGIDELI, MICHAEL WIMMER, Universitaet Regensburg, SAVAS BERBER, DAVID TÓMANEK, Michigan State University, KLAUS RICHTER, Universitaet Regensburg — We investigate spin conductance in zigzag graphene nanoribbons and propose a spin injection method based only on graphene. Combining density functional theory with tight-binding transport calculations, we find that nanoribbons with asymmetrically shaped edges show a non-zero spin conductance and can be used for spin injection. Furthermore, we show that nanoribbons with rough edges exhibit mesoscopic spin conductance fluctuations with a universal value of rmasG ≈ 0.4e/4τ.

8:36AM H29.00004 Electron Transport in Graphitic Nanostructures, PHILIP KIM, Columbia University — Local control of the electrostatic potential in graphene nanostructures can provide a new insight into Dirac fermions in confined geometries in electric and magnetic fields. In this presentation, we report electronic transport measurements in patterned locally gated graphene nanoconstrictions and locally gated single walled carbon nanotubes with tunable transmission and bipolar heterojunctions. We observe various unusual transport phenomena, such as energy gap formation in confined graphene structures and series of fractional quantum Hall conductance plateaus at high magnetic fields as the local charge density is varied in the graphene heterojunction regions. These observed results can be explained in terms of equilibration of chiral edge states at the heterojunction interfaces, indicating charge polarity dependence of quantum Hall edge state equilibration.

9:12AM H29.00005 ABSTRACT WITHDRAWN —

9:24AM H29.00006 Coulomb blockade effects in graphene nanoribbons, FERNANDO SOLS, Universidad Complutense de Madrid, FRANCISCO GUINEA, ICM-CSIC (Madrid), ANTONIO CASTRO NETO, Boston University — We propose that recent transport experiments revealing the existence of an energy gap in graphene nanoribbons may be understood in terms of Coulomb blockade. Electron interactions play a decisive role at the quantum dots which form due to the presence of necks arising from the roughness of the graphene edge. With the average transmission as the only fitting parameter, our theory shows good agreement with the experimental data.

1Work supported by MECS (Spain) and NSF.
9:36AM H29.00007 Distinct Transport Properties of Mono-Layer and Bi-Layer Graphene Nanoribbons, YU-MING LIN, ZHIHONG CHEN, PHAEDON AVOURIS, IBM T. J. Watson Res. Center — Graphene holds promise for future electronic applications owing to its exceptional carrier mobility and a Dirac-like, massless dispersion relation for charge carriers. Here we report on experimental studies of electrical transport properties of graphene nano-ribbon devices. Graphene nano-ribbons devices, consisting of mono-layer and bi-layer graphene, were fabricated by e-beam lithography and plasma etching process. These nano-ribbon devices exhibit size-dependent transport properties due to quantum confinement at low temperatures. We observed distinct transport behaviors for mono-layer and bi-layer devices, and this may be related to a tunable bandgap that can be induced in bi-layer graphene. In particular, in bi-layer devices, we observed a significantly lower noise level than that of single-layer graphene. These findings provide insight into the intrinsic noise mechanisms in graphene layers and also elucidate the impact of the coupling between the two layers in the bi-layer graphene on transport properties.

9:48AM H29.00008 Transverse Field Effect in Graphene Nanoribbons, KATHRYN TODD, HUNG-TAO CHOU, DAVID GOLDHABER-GORDON, Stanford University — We describe transport measurements on graphene nanoribbon devices with separately addressable side gates. Applying the same voltage to both side gates allows us to resolve the Dirac points in the nanoribbon and in the 2-dimensional graphene lead. In conjunction with the side gates, a back gate allows us to separately tune the nanoribbon and the leads between p-type and n-type. Source-drain measurements illustrate the importance of charging effects in these short nanoribbons. Applying opposing voltages to the two side gates allows us to test predictions about the effect of a transverse electric field in graphene nanoribbons.

1Kathryn Todd acknowledges support from the Intel Foundation. This work was supported by the MARCO/FENA program.

10:00AM H29.00009 High-Bias Electronic Transport in Graphene Ribbon Devices, MELINDA HAN, INANC MERIC, KIN FAI MAK, STEPHANE BERCIAUD, TONY HEINZ, KEN SHEPARD, PHILIP KIM, Columbia University — We present experimental studies of electronic transport in graphene under high electric fields. Graphene ribbon devices with varying widths and lengths are fabricated from mechanically exfoliated single-layer graphene sheets using electron beam lithography followed by oxygen plasma etching. Conductance measurements show a trend of current saturation under high source-drain bias. In addition, we employ micro-Raman spectroscopy simultaneously with transport measurement on the current carrying device in vacuum. We observe an enhancement of the G-band anti-Stokes/Stokes intensity ratio, where the optical phonon temperature is estimated to be over ~500K before device failure.


1Supported in part by NSF Grant DMR-0531159.

10:24AM H29.00011 Rough edges in graphene, VLADIMIR CVETKOVIC, ZLATKO TESANOVIC, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD — Recent progress in fabrication of graphene and the understanding of its properties make the graphene a strong contender for a building block of future electronic devices. We analyze the effects of the scattering off rough edges on the transport in graphene nanoribbons. The confinement of the Dirac particles in a nanoribbon is achieved either by means of a large mass term in the Hamiltonian or by imposing boundary conditions appropriate for graphene sheets on the quantum mechanical wave-functions. Variations in the nanoribbon width lead to a nontrivial lateral channel-mixing and provide important limitations to quantum transport. We present a perturbative solution for the problem and derive experimentally measurable conductivity up to the leading order in the case of a nanoribbon with such randomly varying width.

10:36AM H29.00012 Ab initio study of edge functionalization effects on electronic transport through graphene nanoribbons, AMIR FARAJIAN, Wright State University, NARJES GORJIZADEH, YOSHIYUKI KAWAZOE, Tohoku University — We investigate quantum transport through graphene nanoribbons with and without hydrogen saturation. Both armchair-edged and zigzag-edged ribbons with and without hydrogen saturation are considered. For calculating transport properties, we make use of ab initio electronic structure calculations followed by Green’s function implementation of the Landauer’s formalism. The calculated conductance characteristics show significant dependence on the edge functionalization, i.e., whether or not the armchair and zigzag nanoribbons are saturated by hydrogen atoms. The effects of the carrier spin orientations are also discussed. These results are useful in interpreting the experimental data, and in using functionalized graphene nanoribbons for nanoelectronics and sensor applications.

10:48AM H29.00013 Thermoelectric effects in ballistic graphene ribbons, EDUARD BOGACHEK, IGOR ROMANOVSKY, UZI LANDMAN, School of Physics, Georgia Inst. of Technology — A theoretical analysis of electrical and thermal transport in ballistic graphene strips and carbon bilayers, connected to electrodes, is presented. Gate voltage and temperature dependences of thermoelectric coefficients and thermocurrent due for different ratios of strip lengths and widths are studied both in the linear and nonlinear regime (finite applied voltage and temperature differences). Violation of the Onsager relation between the Peltier and thermopower coefficients in the nonlinear regime is considered. Results obtained for carbon bilayers are compared with those in single layers. The effect of transverse voltage applied between layers on the thermoelectric transport in carbon bilayers is investigated.

1Supported by the US D.O.E. (FG05-86ER-45234)

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H30 DCMP: Electronic Properties of Graphene and Related Structures II Morial Convention Center 222
8:00AM H30.00001 Electronic structure of graphene in the presence of disorder¹, ALEXANDER KEMPER, MANOJ SRIVASTAVA, HAI PING CHENG, University of Florida, Gainesville — Graphene, a single layer of the carbon structure graphite, has a number of interesting electronic properties. To aid in the understanding of these properties we have performed first-principles calculations of single graphene layers in the presence of disorder of various forms, including single and double vacancies, Stone-Wales defects, and metallic dopants. We report the effects of defects and dopants on the charge density and electronic density of states. Furthermore, we discuss energetics of these systems and defect-induced spin-states.

¹DE-FG02-97ER45660 & DE-FG02-02ER45995

8:12AM H30.00002 Density of states in graphene with charged impurities¹, BEN YU-KUANG HU, University of Akron, E. H. HWANG, S. DAS SARMA, University of Maryland — We discuss the density of states of graphene in the presence of charged screened impurity scattering. The density of states is obtained from the imaginary part of the single-particle Green’s function, which is evaluated in the Born and the self-consistent Born approximations, and the screened Coulomb impurity potentials are evaluated within the random phase approximation. The density of states in the presence of impurities is typically larger than that of clean graphene at any given energy. In particular, the density of states at the Dirac point, which is zero in a clean sample, becomes non-zero, with a magnitude that is given by an expression akin to that for the BCS superconducting gap.

¹Supported by ONR

8:24AM H30.00003 Topological Frustration in an Alkali-Graphene-Halogen System, YOUJIAN TANG, VINCENT CRESPI, Physics Department, Penn State University — We theoretically studied a system with alkali and halogen adsorbed to opposing sides of a graphene sheet, their mutual interactions then being modulated and constrained by the interposing presence of the sheet. Charge transfer from alkali to halogen generates a substantial dipole moment and large local electric field. Trends with respect to electron affinity, ionization energy, areal density, and the character of the bounding layer (i.e. BN versus graphene) will be discussed.

8:36AM H30.00004 Energy gaps and Stark effects in boron nitride nanoribbons, CHEOL-HWAN PARK, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley, Berkeley, CA 94720 — Graphene nanoribbons, which have been recently synthesized, are regarded as promising candidate materials for nanoscale electronics. It is expected that boron nitride nanoribbons may be produced in a similar way. Notwithstanding their structural similarity, the electronic properties of boron nitride nanoribbons are qualitatively different from those of graphene nanoribbons. Here, we present first-principles calculations of the electronic properties of boron nitride nanoribbons with widths up to 10 nm both without any external potential or under a transverse electric field. The results show a rich set of behaviors and promise for possible applications of boron nitride nanoribbons in nanoscale electronics.

This work was supported by the NSF under Grant No. DMR07-05941, and the U.S. DOE under Contract No. DE-AC02-05CH11231. Computer time was provided by NERSC and NPACI.

8:48AM H30.00005 Band Engineering in C/BN Super-stripes, JEFFREY MULLEN, MARCO BUONGIORNOR- NARDELLI, North Carolina State University — Using electronic structure calculations from first principles, we have studied the electronic characteristics of graphene/BN sheets in a planar “super-striped” geometry. Similarly to Hydrogen-terminated graphene nanoribbons, also C/BN super-stripes show a variation of band gaps associated with the stripe size. Moreover, the bonding with BN introduces confinement effects that can be potentially exploited to enhance the electronic transport properties of these systems. We have characterized these effects by evaluating the band offsets and the electrostatic potential profile across the super-stripe structures.

9:00AM H30.00006 Selective nesting and sensing of molecules on optimally modified material surfaces, JOHN RUSSELL, BOYANG WANG, PETR KRAL, University of Illinois at Chicago, PROF. KRAL’S RESEARCH GROUP TEAM — We develop a methodology of optimal modifications of material surfaces allowing us to design selective nesting sites for inorganic, organic and biological molecules [1]. The idea is to modify material surfaces by atomic dopants and charged ligands in such a way that the created local electric fields form selective Coulombic traps for the adsorbed molecules. We demonstrate this methodology by molecular dynamics simulations of short peptides docked in nesting sites designed on graphene sheets substitutionally doped with B and N atoms. We show that the same approach can be used to selectively dock proteins in water solvent on graphene layers modified by short charged ligands. As a practical application of this methodology, we design and model chemical sensors that could detect the selectively nested molecules. The detection is realized by evaluating the change of the electrical conductivity of the graphene sheets upon the docking of the molecules. [1] B. Wang and P. Kral, Small, 3, 580, (2007). [2] J. Russell, B. Wang and P. Kral, in preparation.

9:12AM H30.00007 Anisotropic Electron-Phonon Coupling on Graphene-Derived Fermi Surface in CaC₆¹, TONICA VALLA, J. CAMACHO, Brookhaven National Laboratory, Z-H. PAN, A.V. FEDOROV, Lawrence Berkeley National Laboratory, A.C. WALTERS, C.A. HOWARD, M. ELLERBY, University College London — Superconductivity in graphite intercalated compounds had been studied for more than 40 years and it is still not fully understood, despite the recent progress and the discovery of relatively high Tc superconductivity in CaC₆ and YbC₆. Initially, even unconventional mechanisms, such as excitonic and plasmonic pairing were considered, but recent studies now suggest that superconductivity in graphite intercalated compounds is more conventional and that the electron-phonon coupling is responsible for pairing. However, it is still not clear whether the graphene-derived electronic states and vibrations or the intercalant-derived ones play more important role, or if some particular combination of graphene-intercalant states and vibrations dominates the coupling. Here, we present angle-resolved photoemission studies of electronic structure in CaC₆. We find that the electron-phonon coupling on the graphene-derived Fermi surface is very strong and anisotropic, reflecting the interaction of graphene-derived states with high-frequency graphene-derived vibrations.

¹This work was supported by the DOE under contract number DE-AC02-98CH10886

9:24AM H30.00008 Fractional statistics of topological defects in graphene and related structures¹, BABAK SERADJEH, MARCEL FRANZ, University of British Columbia — We show that fractional charges bound to topological defects in the recently proposed time-reversal-invariant models of spinless fermions on the honeycomb lattice with Kekule distortion and on the n-flux square lattice with Peierls distortion obey fractional statistics. The continuum effective low-energy description is given in terms of a “doubled” level-2 Chern-Simons field theory, which is parity and time-reversal invariant and implies two species of semions (particles with statistical angle ±π/2) labeled by a new emergent quantum number that we identify as the fermion axial charge.

¹Work supported by NSERC, CIAR, NSF and the Killam Foundation.
of 2 MeV. Motivated by this experiment, we tested interaction between an Ar $^+$ not the structural change but electronic excitation. An experiment [2] showed fluorescence from Ar A highly-charged-ion interacting with graphite causes structural change in nano-scales [1]. While when the ion's kinetic energy reaches few MeVs, the induced is voltages. The behaviour of the gap is discussed as a function of both attractive interaction strength and filling for various graphene-reservoir couplings and in graphene is formulated using the Keldysh path integral formalism, and we obtain generalized gap and number density equations valid for both zero and finite quantum phase transition that occurs at half-filling in equilibrium graphene with attractive interactions. Our system consists of a graphene sheet sandwiched in graphene+nanoparticles system. We find that covered nanoparticles interact weakly with graphene, and that the main effect of the nanoparticles on the electronic structure of graphene is a doping effect that can be modified with the application of an electric field perpendicular to the graphene plane. The system is always metallic, without the opening of a bandgap, even if the nanoparticles are charged: neither the Coulomb potential nor the weak nanoparticle-graphene interaction is able to break the graphene sublattice symmetry. In contrast, in the case of deposited bare (non-covered) Au nanoparticles, there is a relatively strong interaction between low-coordinated Au atoms and graphene carbon atoms beneath. This leads to a symmetry breaking of the graphene sublattices and to the opening of a small bandgap of a few tens of meV.

This work is supported by the Next Generation Supercomputing Project, MEXT, Japan, and by NSAF 10676025.

10:00AM H30.00011 ABSTRACT WITHDRAWN

10:12AM H30.00012 Possible bandgap opening in graphene due to deposited Au nanoparticles: First-principles calculations, RONALDO J.C, BATISTA, SABRINA S. CARARA, HELIO CHACHAM, Universidade Federal de Minas Gerais, Brazil — We perform first-principles calculations to investigate electronic and structural properties of graphene with a layer of deposited Au nanoparticles. We consider Au$_{18}$ nanoparticles that can be either covered with methylthiol molecules, or not. We also consider that the nanoparticles are arranged in a hexagonal lattice, and we focus on the effect of net charge, applied electric fields, and molecular coverage on the electronic structure of the graphene+nanoparticle system. We find that covered nanoparticles interact weakly with graphene, and that the main effect of the nanoparticles on the electronic structure of graphene is a doping effect that can be modified with the application of an electric field perpendicular to the graphene plane. The system is always metallic, without the opening of a bandgap, even if the nanoparticles are charged: neither the Coulomb potential nor the weak nanoparticle-graphene interaction is able to break the graphene sublattice symmetry. In contrast, in the case of deposited bare (non-covered) Au nanoparticles, there is a relatively strong interaction between low-coordinated Au atoms and graphene carbon atoms beneath. This leads to a symmetry breaking of the graphene sublattices and to the opening of a small bandgap of a few tens of meV.

10:24AM H30.00013 Nonequilibrium-induced metal-superconductor quantum phase transition in graphene, SO TAKEI, YONG BAEK KIM, University of Toronto — We study the effects of dissipation and time-independent nonequilibrium drive on an open superconducting graphite monolayer, or graphene. In particular, we investigate how dissipation and nonequilibrium effects modify the semi-metal-BCS quantum phase transition that occurs at half-filling in equilibrium graphene with attractive interactions. Our system consists of a graphene sheet sandwiched by two semi-infinite three-dimensional Fermi liquid reservoirs, which act both as a particle pump/sink and a source of decoherence. A steady-state charge current is established in the system by equilibrating the two reservoirs at different, but constant, chemical potentials. The nonequilibrium BCS superconductivity in graphene is formulated using the Keldysh path integral formalism, and we obtain generalized gap and number density equations valid for both zero and finite voltages. The behaviour of the gap is discussed as a function of both attractive interaction strength and filling for various graphene-reservoir couplings and voltages.

3 This work is supported by the Next Generation Supercomputing Project, MEXT, Japan, and by NSAF 10676025.

10:36AM H30.00014 Detecting single graphene layer by using fluorescence from high-speed Ar$^{7+}$ ion, YOSHIYUKI MIYAMOTO, Nano Electronics Res. Labs. NEC, HONG ZHANG, School of Physical Science and Technology, Sichuan Univ. — A highly-charged-ion interacting with graphite causes structural change in nano-scales [1]. While when the ion’s kinetic energy reaches few MeVs, the induced is not the structural change but electronic excitation. An experiment [2] showed fluorescence from Ar$^{7+}$ ions penetrating through carbon foil with kinetic energy of 2 MeV. Motivated by this experiment, we tested interaction between an Ar$^{7+}$ ion and a graphene sheet by the time-dependent density functional approach, and found that the electronic excitation in the Ar$^{7+}$ ion is also the case even when the incident kinetic energy is 500 KeV and the target thickness is only mono-atomic layer. This simulation suggests the possibility of detecting a suspended mono-atomic layer of graphene [3] by monitoring fluorescence from the penetrated Ar$^{7+}$ ions. We will discuss its importance for analyzing bombardment of solids by highly charged, high-speed ions and possible experiments according to the present result. References: [1] T. Meguro, et al., Appl. Phys. Lett 79, 3866 (2001). [2] S. Baskin, H. Oona, E. Veje, Phys, Rev. A25, 417 (1982). [3] J. Mayer et al., Nature (London), 446, 60 (2007).


Tuesday, March 11, 2008 8:00AM - 11:00AM – Session H31 DMP DCOMP: Focus Session: Computational Nanoscience III: Ferroelectrics, Surfaces, and Water Morial Convention Center 223
8:00AM H31.00001 Properties of Ferroelectric Nanostructures\textsuperscript{1}, INNA PONOMAREVA, Physics Department, University of Arkansas — Ferroelectric nanostructures (FENs) such as thin films, nanowires and nanodots are receiving a lot of attention due to their potential for technological applications and to the rich variety of underlying physics. Interestingly, properties of FENs can substantially deviate from their bulk counterpart due to their sensitivity to many factors. Examples of such factors are the electrical boundary conditions (associated with the full, partial or non-existent screening of polarization-induced surface charges) and mechanical boundary conditions (arising from the lattice mismatch between the FEN and its substrate).

Here, we developed and used computational schemes to predict many properties in various FENs, as well as, to provide atomistic insight to their complex phenomena. In particular, we will show the striking following features and reveal their origins:

- The interplay between electrical boundary conditions, mechanical boundary conditions and growth direction results in the appearance of novel dipole patterns and new low-symmetry phases possessing superior dielectric properties in ferroelectric dots, wires and films\textsuperscript{[1,2]}.
- FENs can exhibit dielectric anomalies, such as a negative dielectric susceptibility\textsuperscript{[3]}.
- Nanobubbles can form in ferroelectric films under an external electric field\textsuperscript{[4]}.
- An homogeneous electric field can be used to control the chirality of vortex structures in asymmetric ferroelectric dots, via the creation of original intermediate states\textsuperscript{[5]}.

\textsuperscript{1}These works are supported by NSF grants DMR-0404335, DMR-0080054 (C-SPIN) and DMR-0701558, by ONR grants N00014-04-1-0413, N00014-03-1-0570, and N00014-01-1-0365 (CPD), and by DOE grant DE-FG02-05ER46188.

8:36AM H31.00002 Internal electric field effects in ferroelectric nanostructures\textsuperscript{1}, BYOUNGHAK LEE, ZHENGJI ZHAO, LIN-WANG WANG, Lawrence Berkeley National Lab — A ground state dipole moment of ferroelectric nanostructures is a long-standing problem. A permanent dipole moment can alter optical and electronic properties of nanostructures, causing state localizations and electron hole separations. A dipole moment in the bulk can have a self-screening effect. In a nanostructure, the different shape of the system can result in an effective screening different from the bulk. In ferroelectric nanostructures, this can lead to a shape dependent total dipole moment, different from the volumetric result derived from its bulk value. Direct ab initio theoretical study on the nanostructure dipole moment is scarce due to the large computational cost. We present a first principles study of this problem using a recently developed Linear Scaling 3-Dimensional Fragment method. We investigated shape and size dependence of the electric dipole moment in various ferroelectric nanorods. We compared our results with experiments and provided an insightful physical picture by analyzing the ab initio numerical results with a classical dielectric model.

\textsuperscript{1}This work is supported by DOE/BES, DE-AC02-05CH11231. It used the resources of National Center for Computational Sciences (NCCS) and National Energy Research Scientific Computing Center (NERSC).

8:48AM H31.00003 Nanowettability by saline solutions in electric field\textsuperscript{1}, ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University (VCU), 1001 West Main Street, Richmond, VA 23284-2006, C.D. DAUB, D. BRATKO, Department of Chemistry, VCU — Molecular simulations of nanosized aqueous droplets and films next to apolar surfaces show a remarkable sensitivity of water contact angles on the applied electric field polarity and direction relative to the liquid/solid interface. We explain the effect by analyzing the influence of the field on interfacial hydrogen bonding which in turn affects the interfacial tensions. When electric field is applied on the aqueous film in the direction perpendicular to the confining hydrophobic surfaces, the competition between field-induced alignment and orientational preference of interfacial water molecules relative to the surfaces results in asymmetric wettability of opposing surfaces (Janus interface). The observed anisotropy in droplet or film wetting is a new nanoscale phenomenon that has so far been elusive as, in current experimental setups, surface molecules represent a very low fraction of the total number of molecules, affected by the field. We discuss amplification of these effects in saline solutions. The work gives basic understanding of field charge effects that can modulate local hydrophilicity of engineered and biological interfaces, as well as surface manipulation in nanofluidic devices.

\textsuperscript{1}Supported by NSF.

9:00AM H31.00004 Electric Field Control of Structure, Dimensionality and Reactivity of Gold Nanoclusters Supported on Thin Films of MgO/Ag(100)\textsuperscript{1}, BOKWON YOON, UZI LANDMAN, Georgia Institute of Technology — External electric field control and manipulations of the structural stability, dimensionality, and chemical reactivity of gold nanoclusters deposited on MgO films grown on an Ag(100) substrate, are introduced and illustrated with the use of first-principles electronic structure calculations. Field-controlled interfacial charging and field-induced structural dimensionality crossover are predicted; These structural changes are accompanied by variations of the chemical reactivity of the adsorbed gold nanostructures.

\textsuperscript{1}Research supported by the US AFOSR and the US DOE. Computations performed at the Georgia Tech Center for Computational Materials Science and the National Energy Research Computational Center (NERSC).
9:12AM H31.00005 Adsorption of water on anatase TiO$_2$ nanoparticles: the role of a wire of undercoordinated Ti sites. 1, M. POSTERNAK, A. BALDERESCHI, EPFL-Lausanne, Switzerland, B. DELLEY, Paul Scherrer Institut, Switzerland — Presence of hydroxyl groups is known to be an important element for the initial integration of titania-coated implants in natural tissues. The existence of OH$^-$ radicals due to water dissociation is indeed responsible for major changes in their surface reactivity, and depends in particular on the preparation of the surface. The stable phase for nanoparticle-sized microstructures is anatase, and crystallites are expected to expose different surface terminations and edges. In this work, we study water adsorption on a model system, consisting of an edge along the [11T] direction, at the intersection of two major (101) surfaces. Using the DMO3$^2$ approach within DFT, we find that water dissociative adsorption occurs at the four-fold coordinated Ti atoms present on this edge, in contrast with the case of the unreactive (101) surface. These results provide evidence of an increased chemical activity of such binding sites for adsorption of atoms and molecules. The mechanisms of the hydroxilation process are discussed in terms of the geometric arrangement, coordination numbers, and acidic/basic character of the relevant Ti and O sites.

1This work is supported by a grant from the ITI Foundation for the Promotion of Implantology, Switzerland.


9:24AM H31.00006 Characterization of Anatase Nanoparticles Using Tight Bonding DFT Simulation . HONG WANG, NING MA, HAO WANG, JAMES P. LEWIS, Department of Physics, West Virginia University, CONDENSED MATTER COMPUTATIONAL GROUP TEAM — The structure and electronic properties of anatase nanoparticles with size ranging from 1.5nm to 2.4 nm have been presented in this paper under ab initio Density Functional Theory computational method. Based on the relaxed structures obtained in our calculation, we propose that the portion of surface in the whole structure effects the geometric configuration of anatase nanoparticles. However, as long as the nanoparticles grow bigger, this affection decreases obviously. The analysis of the frontier orbitals of the nanoparticles in our work make us believe that the frontier orbitals (so called HOMOs) are mostly localized on some corner positions of the whole structure. These corner positions are consist of 4-coordinated Ti atom lack of bridge oxygen atoms. When we adsorb water molecule on different positions on the facets of the smallest particle (TiO$_2$)$_{14}$, it turns out the corner position where the frontier orbitals are mostly localized are most energetic favorable adsorption position for water molecule. These special corner positions will likely act as high attractive spots for the external molecules existing in the nanoparticles’ environment.

9:36AM H31.00007 Single oxide overlayers grown on top of another oxide: Their stability, interaction with metal nanoparticles, and contribution to catalytic activity . SERGEY RASHKEEV, Idaho National Laboratory — Oxides are widely used as catalysts as well as supports for catalytically active metal nanoparticles. The catalytic activity of the system depends on many different factors such as anchoring, sintering, decomposition, and diffusion of metal atoms/clusters on the oxide surface. Here we use a combination of first-principles density-functional calculations and molecular dynamics simulations to investigate how all of these factors may change when the surface of the oxide support is modified by an additional single overlayer of another oxide positioned on it. In particular, we found that deposited monolayer oxide films may show instabilities that result in formation of strong anchoring sites for metal atoms/clusters. Also, an atomic-scale roughness introduced in such a way may slow down the surface diffusion processes and inhibit nanocluster growth/sintering. For example, a single layer of SiO$_2$ on a TiO$_2$ substrate may significantly increase the stability of Au nanoparticles and the efficiency of the catalytic CO oxidation. The author thanks Dr. Steven Overbury (Oak Ridge National Laboratory) for attracting his attention to this problem and INL Laboratory Directed Research and Development program and the U. S. Department of Energy, Office of Nuclear Energy under DOE Idaho Operations Office Contract DE-AC07-05ID14517 for financial support.

9:48AM H31.00008 Role of hydrogen on catalytic reduction of nitric oxide on selected transition metal surfaces . FAISAL MEHMOOD, ANAND U. NILEKAR, MANOS MAVRIKAKIS, University of Wisconsin-Madison — Self-consistent periodic DFT-GGA calculations are used to investigate the NO reduction reaction in presence of atomic H on seven close-packed transition metal surfaces namely, Cu(111), Ag(111), Pd(111), Pt(111), Rh(111), Ir(111), and Ru(0001). The chemisorption of atomic (N, O, H) and molecular (NO, NH, OH, HNO, HNOH, H$_2$NO) reaction intermediates has been systematically studied on each metal surface and the preferred sites and binding energies are determined for a 1/4 ML surface coverage. The activation energy barriers for the relevant set of reactions have also been calculated. Based on these results, the potential energy surfaces (PESs) for direct and H-assisted NO reduction reaction on all the metal surfaces have been constructed. These PESs are used for elucidating the trends for various elementary steps involved in the NO reduction reaction, across the periodic table. These PESs indicate that on (111) surfaces of Cu, Ag, Pd and Pt, H assisted NO reduction is quite favorable by either NOH or HNO reaction intermediate. For remaining three close-packed metal surfaces, i.e. Rh, Ir and Ru we do not find significant change due to presence of H. We also find that the presence of extra H may contribute in formation of HNOH or H$_2$NO on the surface that cause barrier to reduce even further.

10:00AM H31.00009 First-principles study of surface stresses induced by target-receptor interactions on a cantilever sensor . VARADHARAJAN SRINIVASAN, Computational Nanoscience Group, Univ. of California, Berkeley, GIANCARLO CICERO, Dept. of Physics, Polytechnic of Torino, JEFFREY C. GROSSMAN, Computational Nanoscience Group — Nanoscale cantilevers have shown great promise as ultrasensitive, low-power chemical sensors based on the surface stresses induced by interactions between the target species and the receptor coating layer. However, the basic mechanism of these induced stresses is yet to be fully understood, and it is therefore of great fundamental and practical interest to elucidate their electronic and structural origins via the weak interactions that lead to cantilever deflection. An example of such a device is the Au-SiN$_x$ cantilever sensor using functionalized long-chain alkanethiols as a coating layer. Even though the target-receptor interactions are often weak, the induced stresses are quite sensitive to the chemistry of the interacting species. Taking water molecules as a model target and either H- or ω-hydroxy and ω-carboxy alkanethiols as the receptor layer on a Au(111) surface, we use first-principles surface stress calculations to provide a detailed atomistic-level understanding of the various contributions leading to the deflection of a cantilever.

10:12AM H31.00010 Atomic motion and electronic structure of alkanethiol monolayer covered gold surfaces . SABRI ALKISI, HAI-PING CHENG, JEFFREY KRAUSE, University of Florida — Self-assembled alkanethiol monolayers are subjects of great interest because of potential applications in future nano-electronics. In this talk, we report our recent studies of the motions of Au atoms on alkanethiol monolayers using molecular dynamics in conjunction with first-principles calculations. Guided by accurate quantum mechanical calculations, we have calibrated the interactions between Au atoms and monolayers for classical simulations. We then investigate the motions of Au atoms as a function of coverage and temperature. Simulations with improved potential parameters show a good agreement with experimental observations. In addition, we discuss the electronic structure and charge transfer at the interface between the molecular monolayer and gold (111) surfaces.

1DOE: DE-FG02-02ER45995
under the Center for Science and Engineering of Materials at Caltech.

3 channel and the surface quality of the Alq heterostructures. Moreover, conductance maps for biased voltages above the Alq metal. In contrast, using STM in the tunneling mode we can determine the ballistic charge transport length by varying the Alq addition, we can compare the Alq transport has been studied in Fe/Si(001) Schottky diodes using ballistic electron emission microscopy. Spin dependent scattering of polarized ballistic electrons

 Overall, the average stretching mode vibrational frequency increases with decreasing hydrogen bonding density. This density depends strongly on temperature. The water dissociation percentage at the surface can be correlated with the ratio between the weights of the stretching and the bending modes. Our results are in good agreement with inelastic neutron scattering measurements done on wet titania nanoparticles.

Tuesday, March 11, 2008 8:00AM - 11:00AM –
Session H32 GMAG DMP: Focus Session: Magnetic Imaging  Morial Convention Center 225

8:00AM H32.00001 Measuring Spin Dependent Hot Electron Transport Using Spin-Polarized Ballistic Electron Emission Microscopy, VINCENT LABELLA, The University at Albany, ANDREW STOLLENWERK, Harvard University, JOHN GARRAMONE, EVAN SPADAFORA, ILONA SITNITSKY, JOSEPH ABEL, The University at Albany — Spin polarized ballistic electron transport has been studied in Fe/Si(001) Schottky diodes using ballistic electron emission microscopy. Spin dependent scattering of polarized ballistic electrons injected from an Fe coated Au tip into the Fe films has been shown to affect the BEEM current. The spin dependent attenuation lengths were determined by measuring this effect with Fe thickness and found to be 1.8 ± 0.2 nm for the minority spin electrons and 2.5 ± 0.3 nm for the majority spin electrons at a tip bias of 1.5 eV. In addition, the attenuation lengths were measured as a function of tip bias, which indicated that the Fe/Si(001) interface band structure has an effect on the hot electron transport through the diode. Applications of the SP-BEEM technique to other systems will also be discussed.

8:12AM H32.00002 Magnetic properties of single and bilayer MnGa on GaN(0001) investigated by spin-polarized STM, Y. QI, G. SUN, M. WEINERT, L. LI, University of Wisconsin, Milwaukee — We investigated the magnetic properties of ultrathin GaMn layers grown on GaN(0001) by spin-polarized tunneling microscopy (SP-STM) using an Fe coated W tip. The GaN films are grown by plasma-assisted MBE on 6H-SiC(0001), and exhibit a metallic pseudo-1x1 surface structure, consisting of 2.3 ML Ga on top of the Ga-terminated GaN. At room temperature, Mn deposition on this surface resulted in the formation of GaMn islands, with the second layer islands begin to nucleate before the first layer is completed. With a Fe coated W tip, contrast between odd and even layers is observed, indicating layered antiferromagnetic magnetization of the GaMn layers. When Mn is deposited on the pseudo (1x1) at 200 C, a GaMn (3x3) structure is observed. First principles calculations show that Mn substitution of Ga leads to virtual bound states with bandwidth of 1.5 eV, indicating significant Mn-Ga interactions. As a result, top layer Ga atoms form covalent-like bonds. The Mn and the liberated Ga atoms from the “1x1” form the (3x3) structure, with the adatom on the T site.

8:24AM H32.00003 Localized spectroscopic and topographic studies of heterostructures of OSE/M (OSE: organic semiconductor, M: metal) using scanning tunneling microscopy (STM) and atomic force microscopy (AFM), C. R. HUGHES, M. L. TEAGUE, S. MITROVIC, N. C. YEH, Phys. Dept., Caltech, Pasadena CA — We employ STM with AFM to study the charge transport and domain structures of OSE/M heterostructures fabricated under differing growth conditions [OSE: sublimated tris(8-hydroxyquinoline) aluminum (Alq3), M: paramagnetic Au or ferromagnetic La0.7Ca0.3MnO3 (LCMO)]. Specifically, using STM in the point contact mode we are able to determine the work function of the heterostructures by measuring the differential conductance versus bias voltage. In addition, we can compare the Alq3 resistivity variations for heterostructures prepared under different Alq3 annealing conditions and with Au or LCMO as the metal. In contrast, using STM in the tunneling mode we can determine the ballistic charge transport length by varying the Alq3 thicknesses in the OSE/M heterostructures. Moreover, conductance maps for biased voltages above the Alq3 band-gap provide spatially resolved information for the local conductance channel and the surface quality of the Alq3 film, the latter further compared with the surface morphology taken with AFM. This work was supported by NSF under the Center for Science and Engineering of Materials at Caltech.
8:36AM H32.00004 Current-induced magnetization switching with a spin-polarized scanning tunneling microscope. STEFAN KRAUSE, Institute of Applied Physics, University of Hamburg, Germany — In present data storage applications magnetic nanostructures are switched by external magnetic fields. Due to their non-local character, however, cross-talk between adjacent nanomagnets may occur. An elegant method to circumvent this problem is magnetization switching by spin-polarized currents, as observed in GMR [1] as well as in TMR [2] studies. However, the layered structures of these devices do not provide any insight to the details of the spatial distribution of the switching processes. Spin-polarized scanning tunneling microscopy (SP-STM) is a well-established tool to reveal the magnetic structure of surfaces at spatial resolution down to the nanoscale. Besides, SP-STM takes advantage of a perfect TMR junction consisting of an isolating vacuum barrier separating two magnetic electrodes, which are represented by the foremost tip atom and the sample. Our experiments demonstrate that SP-STM serves as a tool to manipulate the switching behavior of uniaxial superparamagnetic nanoislands [3]. Furthermore, we show how SP-STM can be used to switch the magnetization of quasistable magnetic nanoislands at low temperature \( T = 31 \) K. Besides its scientific relevance to investigate the details of current-induced magnetization switching (CIMS), this technique opens perspectives for future data storage technologies based on SP-STM.


9:12AM H32.00005 Bloch line ‘crystallization’ as intrinsic pinning mechanism in ferrimagnetic YIG films 1. JOHN NEAL, Department of Physics, University of Bath, UK, MILORAD MILOSEVIC, Department of Physics, University of Bath, UK, and Department Fysica, Universiteit Antwerpen, Belgium, SIMON BENDING, Department of Physics, University of Bath, UK, IRINA GRIGORIEVA, ALEXANDER GRIGORENKO, Department of Physics and Astronomy, University of Manchester, UK — The present intense drive to develop current-switched magnetic storage media has lead to a renewed interest in ferrimagnetic garnet films which, for several decades, were the focus of devices exploiting manipulation of magnetic ‘bubbles’. In such uniaxial materials, the appearance of Bloch lines in structured domain walls strongly influences their dynamic properties in an applied magnetic field. Here we show that the static magnetic properties of garnet films can also be profoundly influenced due to crystallization of Bloch lines into a square lattice. When a long range order characterizes the domain wall, the magnetic contribution from the isolation of magnetic domains in an applied field. Even in the pinned regime, ultra-sensitive scanning Hall probe measurements reveal the nanoscale motion of magnetic blocks in the walls comprising an integer number of Bloch-lines. Although the estimated displacements (~25 nm) are very much smaller than the domain period, we observe highly correlated motion across many domain walls, driven by the strongly interacting Bloch line lattice.

1 This work was supported by EPSRC grants No. GR/D034264/1 and No. GR/P02707/1 in the UK.

9:24AM H32.00006 Evolution of magnetic domain reversal with temperature in Co/Pt multilayers observed by magneto-optical Kerr imaging. X.P. XIE, X.W. ZHAO, J.W. KNEPPER, F.Y. YANG, R. SOORYAKUMAR, The Ohio State University — The nucleation and evolution of magnetic domain structures at temperature and magnetic field in Co(4 Å)/Pt(tPt) multilayers with perpendicular anisotropy have been studied by magneto-optical imaging techniques. Relatively large Pt layer thicknesses \( t_{Pt} = 43 \) Å and 63 Å are chosen for this study because the interlayer coupling strength in the multilayers varies from weak at room temperature to strong at low temperature. Kerr imaging during the magnetization reversal processes shows the transformation of domain patterns with temperature, which correlates directly with enhancement of interlayer exchange coupling with decreasing temperature. As the domain period is reduced, the domain wall propagation becomes more and more difficult leading to the conversion from domain-wall-propagation dominated reversal at room temperature to nucleation-dominated reversal at low temperatures. The enhanced interlayer coupling at low temperatures leads to the entire multilayer switching as a single ferromagnet: while at higher temperatures, when the interlayer coupling weakens, quasi-independent layer-by-layer magnetic reversal is observed. The transformation from propagation- to nucleation-dominated magnetic reversal can be understood by the competition between activation energies for domain nucleation and propagation. Zeeman energy and thermal energy.

9:36AM H32.00007 Adding depth sensitivity to photoelectron microscopy using the standing wave/wedge method. FLORIAN KRONAST, BESSY GmbH, Berlin, ALEXANDER KEISER, CARSTEN WIEMANN, IF9, Juelich Research Center, RUSLAN OVSYANNIKOV, BESSY GmbH, Berlin, ANDREA LOCATELLI, Elettra, Trieste, DANIEL BUERGLER, REINERT SCHREIBER, IFF-9, Juelich Research Center, CHARLES FADLEY, UC Davis and LBNL Mat. Sci. Div. — Photoelectron microscopy (PEEM) is by now a well-established technique for studying many types of multilayer or multicomponent structure, including samples of relevance to spintronics, semiconductor technology, and polymer-based materials. The lateral resolution in such microscopes is typically 20 nm, but with the prospect of going down to ca. 1 nm in the near future. However, resolution perpendicular to the surface is limited to ca. 100 nm due to electron optics limitations. Here we demonstrate PEEM using photoelectrons with a standing wave created by soft x-ray reflection from a multilayer substrate, and growing one layer of the sample in a wedge form. This standing wave/wedge method has been demonstrated for the first time in experiments with a PEEM located at BESSY in Berlin.

9:48AM H32.00008 Study of the correlation between structural and magnetic properties of MnAs/Si. S. HEGDE, J. KWON, E. FRASER, H. LUO, Department of Physics, University at Buffalo, SUNY, D.H. LEE, C.R. WIE, Department of Electrical Engineering, University at Buffalo, SUNY, LUN COLLABORATION, WIE COLLABORATION — Ferromagnetic MnAs has been widely studied because of its ferromagnetic properties and structural compatibility with conventional semiconductors. Magnetic properties of MnAs grown on Si(001) vary depending upon the growth conditions. To understand the variations, we carried out experiments using X-ray diffraction, atomic force microscopy (AFM) and magnetic force microscopy (MFM), together with magnetization measurements. For this study, MnAs was grown by molecular beam epitaxy (MBE) on Si(001) and Si(111) substrates. The surface structure of MnAs is correlated with the magnetic properties. For samples with no in-plane anisotropy, both AFM and X-ray diffraction measurements show the coexistence of MnAs with orthogonal orientations. The magnetic domains are very different from those observed in MnAs grown on GaAs(001). Significant differences in surface morphology are observed between MnAs layers grown on Si(001) and Si(111) because of the different orientations of MnAs.

10:00AM H32.00009 Magnetic domains in Nd2Fe14B on various length scales. A. KREYSSLIG, Ames Laboratory; JF, TU Dresden, Germany, R. PROZOROV, Ames Laboratory; Dept. of Physics and Astronomy, Iowa State Univ., C. DEWURST, ILL Grenoble, France, P.C. CANFIELD, Ames Laboratory; Dept. of Physics and Astronomy, Iowa State Univ., R.W. MCCALLUM, Ames Laboratory, A.I. GOLDMAN, Ames Laboratory; Dept. of Physics and Astronomy, Iowa State Univ. — Detailed knowledge about the structure of ferromagnetic domains provides a link between microscopic properties, and macroscopic magnetic response. In the well known, and already widely used compound, Nd2Fe14B, the dimension, shape and arrangement of magnetic domains are still in discussion due to lack of suitable methods to study magnetic domain structures in the bulk and due to the geometric complexity observed on the surface. Here, we demonstrate that domain patterns revealed by quantitative Kerr and Faraday microscopy, exist well below the surface as detected by small angle neutron scattering. At room temperature, the easy-axis magnetic anisotropy yields very complex structures of domains on various length scales. In contrast, the cone-like magnetic anisotropy below 135 K reduces the complexity of the domain arrangement to a more regular and anisotropic structure of much larger domains. As a consequence the bulk magnetization increases due to the significant volume reduction of the domain walls. — The support by U.S. DOE (DE-AC02-07CH11358), DFG (SFB463) and the Alfred P. Sloan foundation is acknowledged.
10:12AM H32.00010 Collective Dynamics and Slow Relaxation of Charge/Spin Density Wave domains in Antiferromagnetic Chromium. OLEG SHPYRKO, University of California San Diego, ERIC ISAACS, Argonne National Laboratory and University of Chicago. JONATHAN LOGAN, HYEKYUNG KIM, University of Chicago, MARTIN HOLT, MICHAEL SPRUNG, ZHONGHOU CAI, ALEC SANDY. Argonne National Laboratory — We present coherent x-ray diffraction and x-ray microscopy measurements of slow fluctuations and relaxation of charge- and spin-density wave domains in antiferromagnetic Chromium. Intensity fluctuations of the coherent x-ray speckle of incommensurate charge density wave satellite, combined with time-resolved x-ray microscopy measurements, reveal the collective nature of the uncharacteristically slow domain wall and phase defect fluctuation as well as non-equilibrium charge- and spin-density wavevector relaxation. The observed dynamics of pinned charge- and spin-density wave condensate in Chromium is similar to other examples of elastic media in presence of quenched disorder, ranging from dynamics of vortex lattices in disordered superconductors and sliding friction to snow avalanches and earthquakes. A particularly interesting analogy is dynamics of soft matter undergoing jamming transition, which show similar compressed exponential relaxation behavior.

10:24AM H32.00011 Color properties, hydrogen bonding and magnetic interactions in (TBA)$_3$[Ni(NCS)$_3$]$^\ddagger$. T. V. BRINZARI, O. A. -I. SWADER, J. L. MUSFELDT, University of Tennessee, C. TIAN, M. -H. WHANGBO, North Carolina State University, J. A. SCHLUETER, Argonne National Laboratory — We investigated the optical and vibrational properties of (TBA)$_3$[Ni(NCS)$_3$] a pentacoordinate Ni compound, and compared the results with the more traditional hexacoordinate analog (TEA)$_3$[Ni(NCS)$_3$]. Based upon electronic structure calculations, color properties of this high spin complex can be understood in terms of the crystal field splitting of the d-orbitals and their strong hybridization with the ligands. Temperature dependent vibrational studies show an additional splitting and softening of some of the modes at low temperature, which indicates enhanced hydrogen bonding between sulfur centers and organic ligands at low temperature as well as weak structural phase transitions.

1This work is supported by the National Science Foundation.

10:36AM H32.00012 Ferrofluid Photonic Dipole Contours. MICHAEL SNYDER, JONATHAN FREDERICK, Department of Engineering and Physics, Murray State University, Murray, KY 42071 — Understanding magnetic fields is important to facilitate magnetic applications in diverse fields in industry, commerce, and space exploration to name a few. Large electromagnets can move heavy loads of metal. Magnetic materials attached to credit cards allow for fast, accurate business transactions. And the Earth's magnetic field gives us the colorful auroras observed near the north and south poles. Magnetic fields are not visible, and therefore often hard to understand or characterize. This investigation describes and demonstrates a novel technique to visualize the magnetic fields. Two ferrofluid Hele-Shaw cells have been constructed to facilitate the imaging of magnetic field lines [1,2,3,4]. We deduce that magnetically induced photonic band gap arrays similar to electrostatic liquid crystal operation are responsible for the photographed images and seek to mathematically prove the images are of exact dipole nature. We also note by comparison that our photographs are very similar to solar magnetic Heliosphere photographs.

1Undergrad paper

10:48AM H32.00013 Magnetic Reversal Time in Open Long Range Systems. FAUSTO BORGONOVI, Dipartimento di Matematica e Fisica, Università Cattolica, via Musei 41, 25121, Brescia, Italy, LUCA CELARDO, Department of Physics, Tulane University, New Orleans, LA 70118, BRUNO GONCALVES, Emory University, Atlanta, Ga 30322, LUCA SPADAFORA, Dipartimento di Matematica e Fisica, Università Cattolica, via Musei 41, 25121, Brescia, Italy — Topological phase space disconnection has been recently found to be a general phenomenon in isolated anisotropic spin systems. It sets a general framework to understand the emergence of ferromagnetism in finite magnetic systems starting from microscopic models without phenomenological on-site barriers. Here we study its relevance for finite systems with long range interacting potential in contact with a thermal bath. We show that, even in this case, the induced magnetic reversal time is exponentially large in the number of spins, thus determining stable (to any experimental observation time) ferromagnetic behavior. Moreover, the explicit temperature dependence of the magnetic reversal time obtained from the microcanonical results, is found to be in good agreement with numerical simulations. Also, a simple and suggestive expression, indicating the Topological Energy Threshold at which the disconnection occurs, as a real energy barrier for many body systems, is obtained analytically for low temperature.

Tuesday, March 11, 2008 8:00AM - 10:48AM –
Session H33 GMAG FIAP DMP: Focus Session: Optical Properties of Magnetic Semiconductors
Morial Convention Center 224

8:00AM H33.00001 Full band structure calculations of optical spin injection in Si and CdSe. JULIEN RIOUX, FRED NASTOS, JOHN E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto — We present a theoretical study of optical electron spin injection (optical orientation) in the bulk semiconductors Si and CdSe from direct optical excitation with circularly polarized light[1]. To describe excitation at energies significantly above the band edge, we use full-zone band structures from pseudopotential calculations. For Si, we find that there can be up to 30% spin polarization from direct transitions. The relatively low symmetry of wurtzite CdSe leads to an orientation dependent spin injection, which can be up to 100% polarized at the band edge. Averaging over crystal orientation gives a 50% spin polarization for band edge excitation.


8:12AM H33.00002 Ultrafast optical injection of magnetization in non-magnetic semiconductors, F. NASTOS, R. NEWSON, H. M. VAN DRIEL, J. E. SIPE, Department of Physics, University of Toronto — We discuss the optical injection of magnetization into a nonmagnetic semiconductor by absorption of circularly polarized light. A microscopic approach, based on Fermi's golden rule and k·p band models, is used to quantify the magnetization-injection rate in GaAs. We find that under usual experiment conditions, relevant to optical orientation, the magnetization-injection rate of holes is approximately 20 times larger than it is for electrons, which reflects the large hole magnetic moment. We then turn to the ultrafast excitation regime and explore the possibility that the injected magnetization can radiate a detectable THz field. Using a phenomenological approach for the magnetization relaxation dynamics, we predict that the THz field from optical orientation is at the limit of current THz detection technology.
8:24AM H33.00003 Direct and non-demolition optical detection of pure spin currents in semiconductors1. R.-B. LIU, Department of Physics, The Chinese University of Hong Kong, J. WANG, Department of Physics, The Chinese University of Hong Kong and Department of Physics, Tsinghua University, B.-F. ZHU, Department of Physics, Tsinghua University — We put forward a scheme of direct and non-demolition measurement of a pure spin current in a direct-gap semiconductor by a polarized light beam, which may be view as a “photon spin current” [1]. The effective coupling between the “photon spin current” and the electron spin current is realized via the spin-orbit coupling in valence bands, but involves neither Rashba effect from structure inversion asymmetry nor Dresselhaus effect from bulk inversion asymmetry. Thus a pure spin current, though bearing no net magnetization, induces Voigt and Faraday rotation of a polarized light beam. For the pure spin current studied in Ref. [2], a light beam, if oblique instead of normal incident, would present Voigt and Faraday rotation in the order of 1 millionth rad in the center region of the sample where the spin current flows without spin accumulation. [1] J. Wang, B. F. Zhu, and R. B. Liu, cond-mat/0708.0881. [2] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science 306, 1910 (2004).

8:36AM H33.00004 Theory of Optical Manipulation of Electron Spin in Semiconductors. ALEXANDER EFROS, Naval Research Laboratory — No abstract available.

9:12AM H33.00005 Carrier Dynamics in Microdisk Photonic Molecules1. FELIX M. MENDOZA, ROBERTO C. MYERS, GREG CALUSINE, ARTHUR C. GOSSARD, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106, XIA LI, B.J. COOLEY, NITIN SAMARTH, Materials Research Institute, Penn State University, University Park, PA 16802 — Semiconductor microcavities offer unique means of controlling light-matter interactions, which may be important in optical communications and for quantum information processing schemes. The cavities under study here are coupled microdisks that behave like “photonic molecules” (PMs) with bonding and antibonding states for the confined photon modes. We study different PM geometries consisting of laterally coupled GaAs/GaAlAs microdisks of both circular and elliptical shape. Steady-state photoluminescence measurements reveal bonding and antibonding modes with distinct polarization characteristics. Additionally, we present direct time-resolved spectroscopy of the carrier and spin dynamics in these structures. The combination of static and dynamic spectroscopies is used to explore the evolution of spin coherence in photonic molecule structures.

9:24AM H33.00006 Ultrafast Coherent Precession of Interfacial Electron Spin in Fe/AlGaAs (001). YICHUN FAN, 1327A, Mount Vernon Avenue, Williamsburg 23185, VA, HAIBIN ZHAO, GUNTER LUPKE, AUBREY HANBICKI, C. LI, BEREND JONKER — Magnetic second harmonic generation (MSHG) is used to selectively study the spin dynamics of the interface magnetization for Fe films on AlGaAs(001) in both the dc and time-resolved domain. The interface spin precession is compared with the bulk Fe precession obtained by MOKE. We find: (a) the coherent precession of the interface magnetization is largely non-collinear to the bulk Fe electron spins even at the picosecond time scale; (b) higher frequency spin precession occurs at the interface than in the bulk; (c) the phase of the interface precession is opposite to that of the bulk at low fields; and (d) the interface and bulk precession exhibit different hysteretic behavior. Model calculations of the field dependence of precession frequencies show a large out-of-plane magnetic anisotropy and a large ratio of in plane uniaxial to cubic anisotropy at the interface, attributed to its tetragonal structure and Fe-As bonding. These may account for the significant reduction in exchange coupling between the interface and bulk magnetization. These effects are studied as a function of Fe film thickness and the corresponding evolution of the anisotropy, as well as for the Fe/Si(001) and Fe/AI2O3 interfaces.

9:36AM H33.00007 Spin galvanic effect between subband of InGaAs/AlGaAs 2DEG. JUNFENG DAI, XIAODONG CUI, The University of Hong Kong, THE UNIVERSITY OF HONG KONG TEAM — We report the electric current induced by optically injected spin current on the vicinity of a crossbar shaped InGaAs/AlGaAs two dimensional electronic gas (2DEG) without external electric or magnetic field at room temperature. The electric current is either both in-ward or both out-ward flowing through the crossbar, while the total Hall voltage or current remains negligibly. The geometric size, temperature and external magnetic field dependence of the electric current have been examined and the corresponding mechanism has been discussed.

9:48AM H33.00008 Manipulating nonlinear optical response from electron spins in a 2D electron gas via exciton injection. SHANNON O’LEARY, HAILIN WANG, University of Oregon — The well-known robustness of electron spin coherences in semiconductors has stimulated intense interest in the use of electron spins in semiconductors for spintronics, quantum information processing, and coherent nonlinear optics. Of special importance to these efforts is the understanding and the manipulation of nonlinear optical processes of electron spins. Here, we report experimental studies of coherent nonlinear optical processes of electron spins in a modulation-doped CdTe semiconductor quantum well. These studies elucidate the important roles of trions and excitons and the underlying manybody interactions in the nonlinear optical process. By exploiting a two-color three-pulse pump-control-probe technique, we demonstrate that nonlinear optical responses of electron spins can be effectively manipulated through the injection of an exciton population at an appropriate time. The manipulation of the nonlinear response takes place without electron spin rotation, providing a new approach for the control and applications of electron spins in semiconductors.

10:00AM H33.00009 Rate equation modeling of semiconductor spin-polarized lasers and diodes1. CHRISTIAN GOTHGEN, ATHOS PETROU, IGOR ZUTIC, SUNY Buffalo — Optically or electrically pumped spin-polarized carriers into semiconductor lasers can provide important advantages as compared to the conventional lasers in which the carriers are unpolarized. Motivated by recent experiments in spin-polarized lasers which demonstrate the feasibility of polarization modulation and threshold current reduction [1,2], we model these structures using rate equations. Our approach allows a direct comparison of the analytical and numerical results applied to the steady-state laser response. In the absence of material gain, our findings describe the behavior of spin-polarized diodes. We calculate the dependence of threshold reduction on the degree of pumped spin polarization and suggest how a change in the spin polarization could provide several useful device functionalities.

1Supported by the US ONR and NSF-ECCS CAREER.
10:12AM H33.00010 Theory of spin-polarized semiconductor lasers\textsuperscript{1}, RAFAL OSZWALDOWSKI, CHRISTIAN GOTHGEN, IGOR ZUTIC, SUNY Buffalo — In semiconductor systems spin-polarized electrons couple to photons with definite angular momentum. This effect is the basis for numerous existing and proposed devices \textsuperscript{[1]}. Quantum-well based Vertical Cavity Surface Emitting Lasers (VCSELs) take advantage of this phenomenon to produce circularly-polarized light by using either optical or electrical pumping \textsuperscript{[2]}. We describe the VCSEL system employing Semiconductor Bloch Equations. We include the influence of spin-orbit coupling and the dependence of dipole matrix elements on carrier’s wavevectors. We reduce this description to an effective four-level model, incorporating such effects as different spin lifetimes for electrons/holes and laser-cavity birefringence. Applying this approach to a spin-polarized system, we calculate the threshold current, the polarization of the emitted light and other relevant quantities. \textsuperscript{[1]} I. Zutic, J. Fabian, S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004). \textsuperscript{[2]} M. Holub et al., Phys. Rev. Lett. 98, 146603 (2007). J. Rudolph et al., Appl. Phys. Lett. 82, 4516 (2003).

\textsuperscript{1}Supported by the US ONR and NSC-ECCS CAREER.

10:24AM H33.00011 Disorder and many-body effects in transport and optical conductivities of diluted magnetic semiconductors\textsuperscript{1}, FEDIR KRYCHENKO, CARSTEN A. ULLRICH, Department of Physics University of Missouri - Columbia — The nature of itinerant carriers in diluted magnetic semiconductors like GaMnAs is a subject of intense current debate. The valence-band picture has been widely used, but recent experimental results suggest that the carriers reside in impurity bands. Theoretical results have not been fully conclusive. Most studies within the valence-band picture treat band structures in detail, while disorder and many-body effects are only treated with simple relaxation time and static screening models. We present a more complete theory for electron dynamics in DMSs, combining a multiband approach to a spin-polarized system, we calculate the threshold current, the polarization of the emitted light and other relevant quantities. \textsuperscript{[1]} I. Zutic, J. Fabian, S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004). \textsuperscript{[2]} M. Holub et al., Phys. Rev. Lett. 98, 146603 (2007). J. Rudolph et al., Appl. Phys. Lett. 82, 4516 (2003).

\textsuperscript{1}Supported by NSF ECS-0523918 and ECS-0524253.

10:36AM H33.00012 Theory for Beats Observed in Optical Orientation Experiments on n-GaAs\textsuperscript{1}, NICHOLAS HARMON, WILLIAM PUTIKKA, Ohio State University, ROBERT JOYNT, University of Wisconsin — At low temperatures in n-type semiconductors optical orientation experiments can create two types of spin states: itinerant states in the conduction band and localized states on the donor sites. These two states will in general have different gyromagnetic ratios, and will thus precess at different frequencies when the system is put into a magnetic field. Strong evidence for two types of spins would be to see beats in optical orientation experiments. We have developed a model in the context of coupled Bloch equations to describe this phenomenon. Unpublished data by Awschalom and Kikkawa on n-GaAs at a temperature of 5 K and in a magnetic field of 6 T show beats. We apply our model to this data and interpret it in terms of spins in a Landau level formed from the conduction band states and localized spins on the donor sites.

\textsuperscript{1}Supported by DOE grant DE-FG02-05ER46213

Tuesday, March 11, 2008 8:00AM - 10:48AM –
Session H35 FLAP: Focus Session: Negative Index Materials III
Morial Convention Center 227

8:00AM H35.00001 Plasmonic metamaterials with tuneable optical properties, ANATOLY ZAYATS, The Queen’s University of Belfast — Negative refraction in metamaterials has recently attracted significant attention due to its possible numerous applications in high-resolution imaging and photolithography with the so-called “perfect lenses,” for electromagnetic shielding (visibility cloak), optical signal manipulation, etc. Among various realizations of negative index materials, plasmonic nanostructures play a prominent role as they allow negative refraction properties to be engineered in the visible and near infrared spectral ranges. The coupling of light to plasmonic modes, that are collective electronic excitations in metallic nanostructures, provides the possibility to confine the electromagnetic field on the sub-wavelength scale and manipulate it with high precision to achieve the desired mode dispersion and, thus, reflection, absorption and transmission properties of the nanostructures. In this talk we will discuss various pathways to control dispersion of the electromagnetic waves in plasmonic metamaterials, including plasmon polaritonic crystals and plasmonic nanorod arrays, and the approaches to active tuneability of their optical properties using optical and electric control signals. Both approaches take advantage of the very high sensitivity of surface plasmon mode dispersion on the refractive index of the dielectric adjacent to metallic nanostructure. Hybridization of plasmonic nanostructures with molecular species exhibiting nonlinear optical response allows the development of metamaterials with high effective nonlinear susceptibility due to the electromagnetic field enhancement related to plasmonic excitations. Signal and control light are then coupled to plasmonic modes that strongly interact via nonlinearity introduced by the hybridization. Concurrently, the use of electro-optically active dielectrics incorporated into plasmonic nanostructures provides the route to control optical signals electronically. Plasmonic metamaterials with tuneable optical properties can be used to control negative refraction and electromagnetic field propagation in various applications in nanophotonics, optoelectronics and optical communications.

8:36AM H35.00002 Tunable plasmonic negative index nanostructures and nanolenses in optical domain\textsuperscript{1}, E.V. PONIZOVSKAYA, A.M. BRATKOVSKY, Hewlett-Packard Labs, Palo Alto — We have designed with means of the use of FDTD method a metamaterial, which is a stack of metallic films with periodic hole arrays separated by dielectric layers (usually called fishnet, FN) to have negative index at IR frequencies. Optical modulation of the effective refractive properties of a FN Ag/Si metamaterial structure in the near-IR range has been confirmed experimentally \textsuperscript{[1]}. Pump excitation of the amorphous Si layer was found to be responsible for the observed modulation of the effective refractive index \textsuperscript{[1]}. We discuss the use of gain material to compensate the losses. Arrays of metallic nanoparticles or holes support individual and collective plasmonic excitations that contribute to surface enhanced Raman scattering (SERS), anomalous transparency, negative index, and subwavelength resolution in various metamaterials \textsuperscript{[2]}. Using the FDTD and a boundary integral method we design 2D plasmonic nanolenses with thousand-fold field enhancement factor that can be used for single-molecule SERS detection. \textsuperscript{[1]} E. Kim, et al., Appl. Phys. Lett. 91, 173105 (2007) \textsuperscript{[2]} E.V. Ponizovskaya, A.M.Bratkovsky, Appl.Phys. A 87, 161 (2007)

\textsuperscript{1}Collaboration: E. Kim, W. Wu, Z. Yu, S-Y Wang, R.S. Williams, Y.R. Shen
8:48AM H35.00003 Novel acoustic surface plasmons on Cu(111)1, KARSTEN POHL, BOGDAN DIACONESCU, University of New Hampshire, LUCA VATTUONE, MARIO ROCCA, Universita di Genoa, Italy — The recent discovery of a fundamentally new sound-like plasmon on a bare metal surface of beryllium introduced a new research direction in the area of plasmonics [1]. While conventional surface plasmons are optical modes and have a finite excitation energy of a few eV, the novel acoustic mode can be excited with very low energies of a few meV. This allows, in principle, for a coupling with visible light for signal processing and advanced microscopies as well as new catalysts on metallic surfaces. In order to show that this novel excitation is a general phenomenon on closed-packed noble metal surfaces, as predicted by our theoretical collaborators [2], we have measured the dispersion of the acoustic surface plasmon on Cu(111) by electron energy-loss spectroscopy for a parallel momentum-transfer range from 0 to 0.15 Å⁻¹. We can report that the dispersion is indeed linear (acoustic) with a slope (sound velocity) in good agreement with theory [2].

1Supported by NSF-SGER-DMR-0753467, CNR, and CNISM.

9:00AM H35.00004 Thickness dependent plasmon excitation and damping in metallic thin films, ZHE YUAN, SHIWU GAO, Department of Applied Physics, Chalmers University of Technology, Gothenburg — We present a theoretical study of collective plasmon excitation and lifetime in metallic thin films using a jellium model [1,2]. The excitation spectra are calculated with linear response theory and time-dependent local density approximation. The plasmon energy dispersion follows qualitatively the classical electrodynamical model. For ultrathin films with a few atomic layers, the collective plasmon resonances evolve into single particle transitions at small momenta. The plasmon linewidth due to Landau damping is found to depend exponentially on the film thickness. Quantum oscillations are found in ultrathin films with a period that is about three times longer than the universal period λp/2 observed in many other quantities. This long period results from the dynamical Friedel oscillations in the collective excitation normal to the films. [1] Z. Yuan and S. Gao, Phys. Rev. B 73, 154541 (2006). [2] Z. Yuan and S. Gao, Surf. Sci. in press.

9:12AM H35.00005 Surface Plasmon Polariton Amplification at Telecommunication Frequencies,1, MURALIDHAR AMBATI, SUNGYUN NAM, DENTCHO GENOV, ERICK ULIN-AVILA, XIANG ZHANG, UNIVERSITY OF CALIFORNIA, BERKELEY. TEAM — Active plasmonics describes the interaction between an active medium and surface plasmons, and it offers a foundation for fundamental studies and an opportunity to expand surface plasmon based applications. In order to overcome the challenges posed by surface plasmons - primarily the metal losses - recent studies have focused extensively on surface plasmon amplification; however, there has been very limited headway from the experimental front. We present an experimental evidence of the amplification of long range surface plasmon polaritons (SPPs) by stimulated emission at telecom frequencies. We design SPP waveguides - thin gold metal strips - embedded in a gain medium, erbium doped phosphate glass. We confirm SPP amplification by showing an increase in the propagation length of surface plasmons in both pulsed and continuous modes. We present the design, fabrication and measurements of the gold SPP waveguides in erbium doped glass. Such structures will be suitable as integrated coupling devices as well as for the study of plasmon-exciton interface in cavity quantum electrodynamics.

1This work is supported by NSF Nano-scale Science and Technology Center (NSEC) under award number DMI-0327077.

9:24AM H35.00006 Novel electromagnetic effective medium based on nanocoaxes1, KRZYSZTOF KEMPA, XIWEN WANG, ZHIFENG REN, MICHAEL J. NAUGHTON, Boston College — A thin film of an opaque material, pierced with an array of subwavelength coaxial nanocavities, decomposes an incident electromagnetic wave into spatially discrete wave components, propagates these components without frequency cut-off through the film, and reassembles them on the far side. The propagation of these wave components is fully controlled by the physical properties of the waveguides and their geometrical distribution in the array. This allows for an exceptional degree of control over the electromagnetic response of this effective medium, with numerous potential applications, including metamaterial functionality enabled in the visible frequency range.

1Supported in part by Solasta Inc.

9:36AM H35.00007 Controlling surface plasmons and local field by two-dimensional arrays of metallic nano-bottles, HEI IU, DANIEL H.C. ONG, JONES T.K. WAN, JIA LI, Chinese University of Hong Kong — In recent years, studies of surface plasmon polaritons (SPPs) have been intensive. It is of great interest to control SPPs with great precision and flexibility. In this talk, we present our recent work on SPPs manipulation by using two-dimensional arrays of bottle-shaped, metallic cavities. We propose that by tuning the geometry of such “nano-bottle” contained in a two-dimensional nano-scale array it is possible to control the resonance frequencies and near field patterns of different SPP modes. The dispersion relations are not sensitive to the sizes and depths of the nano-bottles, but depends strongly on the polarization in particular, by using different polarizations, it is observed that different types of SPPs, either propagating or localized, can be excited independently. Moreover, we attempt to control the local field by closing up the aperture of the nano-bottle. We have found that the local field slowly moves up from the bottom to the neck of bottle by increasing its depth. In addition, the field intensity can be fine-tuned by controlling the topology of the bottleneck, for example, a smaller and thinner neck leads to stronger field intensity. As a result, we believe these nano-bottle arrays are good candidates for making high sensitivity chemical and biological sensors.

9:48AM H35.00008 Inverse Mapping Structures onto Transparency1, KIM F. FERRIS, XIN SUN, PAUL A. WHITNEY, Pacific Northwest National Laboratory — Composite materials have continued to make a number of improvements in physical properties (mechanical moduli), but lag behind in optical responses such as transparency. The hybrid nature of the composite material, particle and host matrix, divides light scattering issues into particle size regimes, where the particle size d >> lambda and approximations such as anomalous dispersion have proven useful, and d<< lambda where more exacting methods are necessary. The real-life difference between the ‘design’ particle size and the practical particle size distribution often finds contributions to light scattering losses from both regimes. Using a ceramic-polymer composite as a case example, we have used black box optimization methods to examine the practical bounds for each regime and to assess design rules. These guidelines suggest limitations for particle morphologies and the optical properties of the component materials.

1The authors gratefully acknowledge financial support from the US Dept of Energy and the Office of Science/ Advanced Scientific Computing Research program.

10:00AM H35.00009 A method for determining refractive indices of epilayers of multi-structure active layer, GAGIK SHMAVONYAN, State Engineering University of Armenia — The refractive indices of bulk and epitaxially grown materials differ. Besides, it is very difficult to experimentally determine and theoretically calculate the refractive indices of compound semiconductor epitaxial layers of quantum hetero-structures, especially the refractive indices of active layer of multilayer compound semiconductor devices. For that reason the precise determination of the refractive indices of epilayers is actual. A new method for the determination of the refractive indices of epitaxially grown compound semiconductor materials of multilayer heterostructure is suggested. This method is a combination of experimental measurements and theoretical calculations. The equipment for the fulfillment of the suggested method is also elaborated.
10:12AM H35.00010 Electromagnetic field distributions of perfect and imperfect cloaks, TAI HANG FUNG, LAI LAI LEUNG, KIN WAH YU, Chinese University of Hong Kong, Shatin, NT, Hong Kong — In this work, based on the ideal cloaking model proposed by Pendry et al. [1], we calculate, by first-principles approach, the electric field distributions of ideal cloaks (both spherical and cylindrical) subject to different external electric field sources. The results show that the external electric field of an ideal cloak remains unperturbed and the field inside the cloaking region vanishes, thus verifying that Pendry et al.’s model is indeed perfect. We then extend the investigation to imperfect cloaks, whose permittivity tensors can be perturbed due to dispersion or loss, by solving the appropriate boundary-value problems [2]. The resultant electric field distributions can become nonzero inside the vertical cantilevers along region as expected. We further evaluate the visibility of the imperfect cloak against the perturbation. We find small visibility under appropriate conditions.


10:24AM H35.00011 Design of cloaking metamaterials using spectral representation theory, LAI LEUNG, TAI HANG FUNG, KIN WAH YU, Chinese University of Hong Kong — Controlling the propagation of electromagnetic (EM) waves, for instance in cloaking problems, has become an important topic in nanophotonics. So far, following the cloaking model proposed by Pendry et al. [1], the experimental realization was only limited to the microwave region [2]. Since practical application lies in the visible range, we have extended the investigation to that region by utilizing nanocomposites with reference to the material parameters proposed by Pendry et al. and Shalaev et al. [3]. The calculations can be made much simpler by invoking the spectral representation theory [4]. The loss and dispersion effects, as well as the propagation of EM waves are assessed for the designed cloaking models in order to investigate the cloaking performance. Further analyses show that our models can accomplish the desired cloaking effect in the visible range. Moreover, the loss and dispersion effects are found to be small and acceptable.


10:36AM H35.00012 Nonlinear Cerenkov radiation in a two-dimensional nonlinear photonic crystal waveguide, S.N. ZHU, Y. ZHANG, Z. YAN, Z. QI, G. ZHAO, National Laboratory of Solid State Microstructures, Nanjing University — We present a new type of quasi-phase-matched Cerenkov radiation generation from a two-dimensional nonlinear photonic crystal waveguide: a hexagonally poled LiTaO3 waveguide. The waveguide was fabricated by field poling followed by proton exchange technique. The fundamental source was a LD-pumped, 90-ns pulsed Q-switch double wavelength Nd:YAG laser at 1064-µm and 1319-µm. The pulse repetition rates was 8-kHz. When the fundamental beams at 1064-µm and 1319-µm were co-linearly focused into the waveguide and propagated along its x-axis, multiple radiation spots at red, yellow, green with different propagation directions and radiation angles are simultaneously exhibited from such a hexagonally poled waveguide. Scattering involved Cerenkov arc is also observed. These frequency conversion processes were realized by guided-to-radiated mode interaction. Phase-matching for these processes in the waveguide was automatically achieved by a quasi-phase-matched Cerenkov configuration.

Tuesday, March 11, 2008 8:00AM - 10:48AM
Session H36 GIMS: Focus Session: Advances in Scanned Probe Microscopy II: Force Methods Morial Convention Center 228

8:00AM H36.00001 Multi-dimensional Scanning Probe Microscopy, HANS J. HUG, Empra, Materials Science and Technology, CH-8600 Duebendorf, Switzerland and Institute of Physics, University of Basel, CH-4056 Basel, Switzerland — Since the first demonstration of atomic force resolution with a scanning force microscope in 1995 a large variety of samples have been imaged with atomic resolution. In 2000 Gießel obtained atomic resolution with a (macroscopic) tuning fork operated with small oscillation amplitudes that correspond to the length of the inter-atomic interaction potentials. However, tuning fork sensors have a number of disadvantages that can all be overcome by optimized micro-fabricated cantilevers operated at similarly small or even smaller oscillation amplitudes. With their small mass and high mechanical quality factor, particularly after appropriate annealing in UHV force sensitivities that are orders of magnitude better than that of tuning forks and also far better than that of the best NEMS sensors is obtained. Recently Kawai et al and Sugimoto et al obtained atomic resolution with cantilevers with a operated in higher oscillation modes with sub-nanometer amplitudes. In order to make use of the excellent force sensitivity we developed a Fabry-Perot type interferometer optical sensor that maps flexural and torsional cantilever oscillations with ultra-high sensitivity. This deflection sensor allows the use of sub-A canrilever oscillation amplitudes and thus the direct measurement of atomic interaction force gradients and, in principle, the use of advanced tunnelling spectroscopy techniques that are well-established in the field of scanning tunnelling microscopy. The simultaneous mapping of flexural and torsional oscillation modes further allows the measurement of vertical and lateral tip-sample interaction forces and corresponding atomic scale energy loss processes.

8:36AM H36.00002 A Low Temperature Scanning Force Microscope with a Vertical Cantilever and Interferometric Detection Scheme, JEEHOON KIM, T.L. WILLIAMS, SANG LIN CHU, HASAN KORRE, MAX CHALFIN, J.E. HOFFMAN, Harvard University — We have developed a fiber-optic interferometry system with a vertical cantilever for scanning force microscopy. A laser, mounted on a Pan-type walker, was used to collect the interference signal in the cavity between the cantilever and the single mode fiber. This vertical geometry has several advantages: (1) it is directly sensitive to lateral forces; (2) low spring constant vertical cantilevers may allow increased force sensitivity by solving the “snap-in” problem that occurs with soft horizontal cantilevers. We have sharpened vertical cantilevers by focused ion beam (FIB), achieving a tip radius of 20 nm. We will show test results of a magnetic force microscope (MFM) with this vertical cantilever system.

1This work is supported by NSF/PHY 01-17795.

8:48AM H36.00003 New Interpretation of Non-contact Atomic Force Microscopy Images of Dihydride Si(001) Surface Based on Simulation, AKIRA MASAGO, SATOSHI WATANABE, The University of Tokyo, KATSUNORI TAGAMI, MASARU TSUKAKA, Waseda University — Dihydride Si(001) surfaces have attracted attention as a substrate of organic semiconductor devices. In non-contact atomic force microscopy (NC-AFM) observation of dihydride Si(001) surface, 1x1 and 2x1 images were observed depending on the preset frequency shift value [1]. For both images, bright spots were assigned to hydrogen atoms. Recently, we have developed a simulator on the basis of the density-functional based tight-binding method, and have simulated NC-AFM image of the dihydride Si(001) surface. As a result, we obtained frequency shift images with the 1x1 and 2x1 periodicities, which agree well with the experiments. Surprisingly, we have found that the bright spots of the 2x1 image do not correspond to hydrogen atoms. Each spot corresponds to the bridge site, where the sum of the attractive forces from two nearby hydrogen atoms becomes large.

10:00AM H36.00009 Fabricating overhanging magnets for use in magnetic resonance force microscopy using a XeF2 isotropic etch. SARAH WRIGHT, Cornell Department of Chemistry and Chemical Biology. STEVEN HICKMAN, JOHN MAROHN, Cornell Department of Chemistry and Chemical Biology — Pushing magnetic resonance force microscopy towards single proton sensitivity demands meeting the nanofabrication challenge of producing an attonewton-sensitivity cantilever with a magnetic tip whose diameter is 50 nm or less. At the same time, the cantilever should also experience low force noise (and force gradient noise) near the sample. As proof of concept, we will show a 50-nm overhanging cobalt magnet made by a process involving KOH etching, as well as preliminary work on making overhanging magnets by FIB micro machining. We have characterized high coercivity Sm2Co17 MRFM probes fabricated by Focused Ion Beam (FIB) micro machining and mounted on a commercial Si cantilever (characteristic dimension 1 mm x 1 mm x 1 mm). We report vibrating cantilever magnetometry measurements of probe coercivity. Low temperature (4 K) probe coercivity as high as 1 T has been observed. Probe characteristics have also been deduced from deconvolution of MFM data obtained on 5.3 μm diameter permallloy dots. We also discuss energy dissipation in the micromechanical cantilever when the tip approaches a ferromagnetic sample.

10:12AM H36.00010 Bimodal AFM imaging of individual protein molecules with sub-pico Newton force sensitivity. NICOLAS F. MARTINEZ, SHIVA PATIL, JOSE R. LOZANO, RICARDO GARCIA, Instituto de Microelectronica de Madrid, CSIC — The capability of atomic force microscopes (AFM) to generate atomic or nanoscale resolution images of surfaces has deeply transformed the study of materials. However, high resolution imaging of biological systems has proved more difficult than obtaining atomic resolution images of crystalline surfaces. In many cases, the forces exerted by the tip on the molecules (1-10 nN) either displace them laterally or break the noncovalent bonds that hold the biomolecules together. Here, we apply a force microscopy concept based on the simultaneous excitation of the first two flexural modes of the cantilever (bimodal excitation). The coupling of the modes generated by the tip-molecule forces enables imaging under the application of forces (around 35 pN) which are smaller than those needed to break noncovalent bonds. With this instrument we have resolved the intramolecular structure of antibodies in monomer and pentamer forms. Furthermore, the instrument has a force sensitivity of 0.2 pN which enables the identification of compositional changes along the protein fragments.

1Partial work was supported by the NSF Grant No. ECS0601571

1We acknowledge the financial support from the European Commission (FORCETOOL) and the MEC (Spain)
10:24AM H36.00011 Rheological Measurements by AFM of the Formation of Polymer Nanofibers, MEHDI YAZDANPANAH, MAHDI HOSSEINI, SANTOSH PABBA, electroOptics Research Institute and Nanotechnology Center University of Louisville, SCOTT BERRY, VLADIMIR DOBROKHOV, ABEDELILAH SAFIR, ROBERT KEYNTON, ROBERT COHN, electroOptics Research Institute and Nanotechnology Center University of Louisville, ELECTROOPTICS RESEARCH INSTITUTE AND NANOTECHNOLOGY CENTER UNIVERSITY OF LOUISVILLE COLLABORATION, DEPARTMENT OF MECHANICAL ENGINEERING COLLABORATION — Polymer fiber can be formed by pulling a thread of polymeric liquid if the fiber solidifies before it breaks up by capillary thinning. Fiber diameter is well correlated with a processing parameter that is a simple function of viscosity, surface tension and evaporation rate. The fundamental material parameters can also be determined with the same AFM setup. The usual problem with tapered AFM tips, of liquids wetting unstably up the tapered AFM tip and even onto the cantilever, is resolved by the use of long cylindrical tips of constant diameter. We recently demonstrated a method of growing Ag-Ga nanowires onto AFM tips at room temperature. These constant diameter nanowires are shown to give clearly measurable force-distance curves when inserted through the surface of a liquid, which provides clean measurements of surface tension, contact angle, and evaporation rate, while shear viscosity is determined through cantilever Q-damping as a function of insertion distance into the liquid.

10:36AM H36.00012 Micromechanical force detectors for measuring magnetization at high magnetic fields and the magnetic response of Ba3Cr2O8, K. NINIOS, Y. J. JO, L. BALICAS, A. ACZEL, G. M. LIKE, H. B. CHAN, DEPT OF PHYSICS, UNIVERSITY OF FLORIDA TEAM, NHMFL, TALLAHASSEE COLLABORATION — We report magnetization measurements of Ba3Cr2O8 using micromechanical faradary balance magnetometers. The magnetometers consist of a movable polysilicon plate (500 by 500 micrometers) supported by four springs 2.75 micrometers above a fixed electrode. When small samples of the magnetic material are placed at the center of the movable plate, the natural gradient of the field creates a force on the sample that can changes the capacitance between the plate and electrode, while the response to magnetic torque is minimized. The absolute magnetization of the sample can be determined provided that the magnetic field gradient is known. The device is used to measure the magnetization of a small sample of Ba3Cr2O8 with mass of 1 microgram. At high fields, our measurements reveal an asymmetrical dome-like structure in the temperature-magnetic field phase diagram, possibly related to the Bose-Einstein condensation of spin triplet degrees of freedom.

Tuesday, March 11, 2008 8:00AM - 10:48AM — Session H37 FLAP: Optical Properties of Semiconductors (mostly oxides) Morial Convention Center 229

8:00AM H37.00001 Density-functional theory study of the effects of atomic doping on the band edges of monoclinic WO3, MUHAMMAD N. HUDA, YANFA YAN, SU-HUAI WEI, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, Golden, CO 80401 — The effects of impurities in room temperature monoclinic WO3 were studied using the local density approximation to density-functional theory. Our main focus is on nitrogen impurity in WO3, where both substitutional and interstitial dopings were considered. We have also considered doping with transition-metal atoms and some co-doping approaches in WO3. We found that, in general, band gap reduction was a common result due to the formation of impurity bands in the band gap. Also, the changes of band-edge positions, valence-band maxima and conduction-band minima, were found to depend on the electronic properties of the foreign atom and their concentration. Our results, therefore, provide guidance for making WO3 a suitable candidate for photo-electrodes for hydrogen generation by water splitting.

8:12AM H37.00002 Materials for Transparent Electronics: Ab initio calculation of wide bandgap semiconductor interfaces, SKYE DORSETT, GUENTER SCHNEIDER, Oregon State University — Materials used in transparent electronics (TE) must be transparent in the visible portion of the electromagnetic spectrum which requires the use of wide bandgap semiconductors as contacts and rectifiers as well as passivation and barrier-shaping layers. Of particular importance are the source and drain contacts of transparent thin-film transistors (TTF). The contact characteristics at the interface between the channel material (e.g. ZnO, SnO2) and the contact material (commonly Indium Tin Oxide) are determined by the band offset which can be estimated from a heterojunction model based on material properties alone. The development of new materials for TE greatly benefits from estimates of interface properties but for most materials which hold promise for use in TE (e.g. indium gallium zinc oxide) the relevant material parameters such as work function, electron affinity and in particular the charge neutrality level are not known. To close this gap we report ab-initio density functional theory calculations of band offsets for wide bandgap semiconductors which are commonly used or hold promise for use in TTF.

8:24AM H37.00003 Ab initio calculations of the dielectric functions of semiconductors including the electron-hole interactions via LASTO method, HYEJUNG KIM, YIA-CHUNG CHANG, University of Illinois at Urbana-Champaign and Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan — We calculate dielectric functions of semiconductors including the electron-hole interactions within the ab initio framework. The Bethe-Salpeter equation is constructed using a full-potential linear augmented-Slater-type orbital (LASTO) method [1, 2]. Using the LASTO method allows us to compute optical matrix element for large number of k points efficiently. Due to requirements of a dense k-point mesh, we use quasi-minimum residual (QMR) method to solve the equation. The inclusion of the electron-hole interactions both shifts the peak positions and changes peak heights of the imaginary part of the dielectric functions, resulting in better agreement with experimental data than the spectra obtained without including the electron-hole interactions. The calculated dielectric functions are compared to experimental data of ZnSe, CdSe, CdTe, InP, InAs, AlAs and GaN. The self-energy correctives are described by an empirical tight-binding formula. [1] J. W. Davenport, Phys. Rev. B 29, 2896 (1984) [2] Y.-C. Chang, R.B.James, and J.W.Davenport, Phys. Rev. B 73, 035211 (2006)

8:36AM H37.00004 Structural and optical properties of a transparent conductor oxide: Nb:In2O3, O. LOZANO, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX, P.V. CHINTA, P.V. WADEKAR, L.H. CHU, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX., H.W. SEO, Department of Physics, University of Alaska, Little Rock, AK, O.Q. CHEN, X.M. WANG, D. WIJESUNDERA, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX., L.W. TU, N.J. HO, Departments of Physics and Materials and Optoelectronic Engineering and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, TW, W.K. CHU, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX. — Thin films of niobium-doped indium oxide, Nb:In2O3, have been deposited on YSZ(001) and MgO(111) substrates by magnetron sputtering at 450 °C. The transparent semiconducting films obtained on YSZ(001) were epitaxial, but when deposited under the same conditions on MgO(111), the film qualities worsen upon Nb doping. The structural and optical properties in relation to the Nb content and the general growth conditions were studied by Rutherford backscattering, ion channeling, optical absorption spectroscopy, x-ray diffraction, and atomic force microscopy. The magneto-transport behaviors will also be discussed.
8:48AM H37.00005 Nature of the bandgap in In$_2$O$_3$ revealed by first-principles calculations and X-ray spectroscopy, ARON WALSH, JUAREZ L.F., DA SILVA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO 80401, USA, CHRISTOPH KÖRBER, ANDREAS KLEIN, Darmstadt University of Technology, Darmstadt, Germany, L.F.J. PIPER, ALEX DEMASI, K.E. SMITH, Department of Physics, Boston University, Boston, MA 02215, USA, G. P Aceccio, J., Laboratorio TASC, INFN-CNR, Area Science Park, 34012 Trieste, Italy, P. TORELLI, CNR-INFN-S3, Via Campi 213/A, I-41100 Modena, Italy, D.J. PAYNE, A. BOURLANGE, R.G. EGDELL, Chemistry Research Laboratory, Mansfield Road, Oxford OX1 3TA, UK — The origin of weak absorption 1 eV below the onset of strong optical absorption in In$_2$O$_3$ has previously been attributed to the presence of an indirect fundamental bandgap or surface band bending. We demonstrate conclusively that this is not the case. Through the application of bulk and surface sensitive X-ray spectroscopic techniques, we reveal that the valence band edge is found much closer to the bottom of the conduction band than expected on the basis of the widely quoted bandgap of 3.75 eV. First-principles theory shows that the upper valence bands of In$_2$O$_3$ exhibit small dispersion and the conduction band minimum is positioned at Γ; however, direct optical transitions give minimal dipole intensity until 0.8 eV below the valence band maximum. Our results set an upper limit on the fundamental bandgap of 2.9 eV.

9:00AM H37.00006 Raman scattering properties of SnO$_2$, RALF MEYER, Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany, CEDRICK MEIER, AXEL LÖRKE, Experimental Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — Oxide semiconductors like ZnO and SnO$_2$ have recently attracted a lot of attention as possible optical materials for novel technological applications. Results from Raman scattering experiments and ab initio calculations of the Raman scattering properties of bulk SnO$_2$ and SnO$_2$-δ have been performed. Raman spectra derived from these calculations compare qualitatively well with the experimental findings. From this, it is concluded that the differences in the experiments are an effect of the bulk materials. An analysis of the nature of the calculated Raman active vibrational modes makes it possible to draw further conclusions on the reasons behind the differences between the stochiometric SnO$_2$ and the understochiometric SnO$_2$-δ.

9:12AM H37.00007 Studies of electronic relaxation and coherent control in sensitized semiconductor surfaces, VICTOR BATISTA, Yale University, LUIZ REGO, Universidade Federal de Santa Catarina (UFSC) — This talk addresses the feasibility of using sequences of unitary pulses for coherent-control of quantum dynamical phenomena, including superecho and tunneling in sensitized TiO$_2$ surfaces and control of tunneling and decoherence in archetypal model systems. The proposed dynamical decoupling scenario is based on the repetitive application of unitary pulses, affecting the interference phenomena between wave-packet components. The pulses affect the overall relaxation dynamics without collapsing the coherent-quantum evolution of the system. It is shown that both bound-to-bound state tunneling and bound-to-continuum tunneling processes can be inhibited and eventually halted with sufficiently frequent pulses that exchange energy with the system but do not collapse the unitary evolution or affect the potential energy tunneling-barriers. The reported results are therefore particularly relevant to the understanding of coherent optical manipulation of electronic excitations in semiconductor devices where performance is limited by quantum tunneling and decoherence.

1Supported by the Deutsche Forschungsgemeinschaft (SFB 445)

9:24AM H37.00008 Electron-phonon interaction and charge carrier mass enhancement in electron doped alkali earth titanate semiconductors, DOOK VAN MECHELEN, DIRK VAN DER MAREL, CLAUDIO GRIMALDI, PETER ARMITAGE, ALEXEY KUZMENKO, HANS HAGEMANN, NICOLAS REYREN, ROLF LORTZ, IGOR MAZIN, University of Geneva, Geneva — We have studied the electron-phonon coupling in electron doped SrTiO$_3$ for which the carrier concentration ranges from a dilute gas of polarons to a polaron liquid. Here we report a THz, far-infrared and optical study together with DC conductivity, Hall effect and specific heat measurements. The THz spectra at 7 K show the presence of a very narrow (< 2 meV) Drude peak, the spectral weight of which shows approximately a factor of three enhancement of the band mass for all carrier concentrations. The missing spectral weight is regained in a broad ‘mid-infrared’ band which originates from electron-phonon coupling. Analysis of the results yields an electron-phonon coupling parameter of an intermediate strength, α ~ 4. Specific heat measurements below 4 K show the mass enhancement to be about eight times the band mass for all carrier concentrations. The outstanding discrepancy with the optical mass is interpreted together with the temperature dependence of the Hall constant, the optical spectral weight and the dc scattering rate within the framework of a polaron liquid.

9:36AM H37.00009 Non-resonant inelastic x-ray scattering spectra of lithiumated titanium oxides for battery applications, KENNETH NAGLE, University of Washington, MALI BALASUBRAMANIAN, Advanced Photon Source, Argonne National Laboratory, CHRISTOPHER JOHNSON, Chemical Engineering Division, Argonne National Laboratory, GERALD SEIDLER, University of Washington, KENNETH NAGLE, University of Washington, MALI BALASUBRAMANIAN, Advanced Photon Source, Argonne National Laboratory, CHRISTOPHER JOHNSON, Chemical Engineering Division, Argonne National Laboratory, GERALD SEIDLER, University of Washington, KENNETH NAGLE, University of Washington, MALI BALASUBRAMANIAN, Advanced Photon Source, Argonne National Laboratory, CHRISTOPHER JOHNSON, Chemical Engineering Division, Argonne National Laboratory, GERALD SEIDLER, University of Washington — Many lithium ions are used in batteries, and for this reason it is important to understand the electronic structure of lithiumated titanium oxides. We present non-resonant inelastic x-ray scattering (NRIXS) spectra from Li$_2$O initial states in TiO$_2$; these spectra are among the first recorded for such states in a transition metal. These spectra were obtained using the lower energy resolution inelastic x-ray scattering (LERIX) spectrometer, which is capable of making simultaneous non-resonant inelastic x-ray scattering (NRIXS) spectra from 2p initial states in titanium; these spectra are among the first recorded for such states in a transition metal. Theoretical calculations have shown that the band mass enhancement to be about eight times the band mass for all carrier concentrations. The results demonstrate the interpretation of experiment, the electronic excitations in semiconductor devices where performance is limited by quantum tunneling and decoherence.

9:48AM H37.00010 New green phosphor Ba$_3$Si$_2$O$_6$N$_2$:Eu for white LED: crystal structure and optical properties, MASAYOSHI MIKAMI, KYOTA UHEDA, SATOSHI SHIMOKA, HIROYUKI IMURA, NAOTO KIJIMA, Mitsubishi Chemical Group Science and Technology Research Center, Inc. — A new oxynitride, Ba$_3$Si$_2$O$_6$N$_2$, has been synthesized. The crystal structure has been successfully determined by close collaboration between experiment and first-principles band calculation based on density functional theory. This compound doped with Eu exhibits intense green photoluminescence with high color purity under near-ultraviolet to blue light excitation. It has much less thermal quenching at room temperature. The optical properties of these compounds have been interpreted from theoretical and crystallographic viewpoint.

10:00AM H37.00011 Optical properties of group-II oxides — excitons and absorption in MgO, ZnO and CdO, ANDRE SCHLEIFE, CLAUDIA RÖDL, FRANK FUCHS, FRIEDHELM BECHSTEDT, Institut fuer Festkoerpertheorie und -optik, Friedrich-Schiller-Universitat and European Theoretische Spectroscopy Facility (ETSF) — ZnO is a material that has been very attractive for researchers for many decades by now. However, recently also alloys and heterostructures with other group-II oxides are becoming more and more interesting. Together with MgO or CdO the tuning of electronic and optical properties becomes possible with potential applications for optoelectronic devices in the blue or UV spectral region. For the three materials we study the influence of excitonic effects on the dielectric function in the region of interband transitions and on the electron-hole binding near the absorption edge by solving the Bethe-Salpeter equation. As starting point we compute the electronic structure using a GGA+U approach. The U is chosen to widely reproduce more sophisticated HSE06+G(W) calculations. We combine two efficient approaches to calculate the spectrum and bound excitonic states, using a large number of k-points in combination with hybrid k-point meshes to ensure convergence. We find good agreement of our challenging ab initio calculations with experimental absorption spectra as well as values for the binding energies.
10:12AM H37.00012 Mechanistic model for the influence of Ag thickness on the electrical and optical properties of ZnO/Ag/ZnO nanoscale multilayers, TERRY ALFORD, HAUK HAN, School of Materials and Flexible Display Center at Arizona State University, N. THEODORE, Analog & Mixed-Signal Technologies, Freescale Semiconductor Inc. In this study, we have engineered TCO structures with greatly improved electrical conductivity by introduction of a thin layer of Ag. Results show that carrier concentration, mobility, and conductivity increase with Ag thickness. The electrical conductivity decreased from 1 Ω-cm to 8×10⁻⁵ Ω-cm for a 14 nm Ag middle layer, by increasing carrier concentration and mobility. AFM and TEM results indicate that low Ag thickness results in Ag island formation. The optical transmittance of the composite structure decreases when compared to a single ZnO layer of comparable thickness. However, we demonstrate that an optimum Ag thickness exists (12 nm) to fulfill the conductivity and transmittance requirements for optoelectronic devices. Moreover the optical band-gap of ZnO/Ag/ZnO composite multilayer films decreases with increasing Ag thickness and also increases with carrier concentration. Based on these results, we propose a mechanistic model for the influence of Ag thickness on the electrical and optical properties of this system.

10:24AM H37.00013 Soft X-Ray Spectroscopic studies of Intrinsic Quantum Well States, Shallow Core Level Hybridization, and Valence Band Structure in CdO and InN1, L.F.J. PIPER, L. COLAKEROL, A. DEMASI, T.D. MOUSTAKAS, K.E. SMITH, Boston University, J. ZUNIGA-PÉREZ, V. MUNOZ-SANJOSÉ, Universitat de Valncia, ALEXEI FEDOROV, Advanced Light Source, LBNL, T. VEAL, C. MCCONVILLE, University of Warwick — InN and CdO are post-transition metal compounds that display significant metal-ligand shallow core level hybridization [1], and have recently been discovered to possess intrinsic quantum well states in electron accumulation layers near their surfaces [2]. We report here new synchrotron-based soft x-ray spectroscopic measurements of the electronic structure of CdO and InN single crystal thin films. Resonant x-ray emission spectroscopy has been employed to study the detailed valence band and shallow core level electronic structure, while high resolution angle-resolved photoemission spectroscopy was used to measure quantized electron subbands at the near-surface of both InN and CdO. [1]. L. F. J. Piper et al., Phys. Rev. B (2007) in press; [2]. L. Colakeroi et al., Phys. Rev. Lett. 97, 237601, (2006)

1 Experiments performed at the ALS and the NSLS. Work supported in part by the Department of Energy and the ACS Petroleum Research Fund.

10:36AM H37.00014 Probing defects in ZnO nanostructures by Photoluminescence and Positron Annihilation Spectroscopy1, MANORANJAN GHOSH, A.K. RAYCHAUDHURI, S.N. Bose National Centre for Basic Sciences, S.K. CHAUDHURI, DIPANKAR DAS, UGC-DAE Consortium for Research — We have investigated defect related emission in the blue green region (2.2 eV - 2.5 eV) of ZnO nanostructures having spherical (5 nm-15 nm) as well as those with hexagonal platelet and rod like morphologies (20nm-100 nm), synthesized by solvo-thermal route. This emission show anomalous size dependence. Emission energy near 2.2 eV, shifts to higher energy (2.5 eV) for increase in size beyond 20nm when shape of the nanostructures changes. This change in photoluminescence has a close correlation with the size (and shape) induced change in the positron trapping rate which is directly proportional to the defect concentration. The trapping rates show non-monotonous dependence on size. It increases initially as the size increases (5nm-15nm) and then decreases as the size increases beyond 20nm. While increase of the trapping rate on size reduction is expected due to accumulation of more defects at the surface, the initial dependence of the trapping rate on the size (below 20nm) is anomalous. The data are explained by the presence of defects like Zn vacancy and confinement due to size reduction.

1 DST Unit for Nanoscience

Tuesday, March 11, 2008 8:00AM - 11:00AM — Session H39 GSNP: Student Prize Session followed by Focus Session: Friction Morial Convention Center 231

8:00AM H39.00001 Restricted Defect Dynamics in Colloidal Peanut Crystals, SHARON GEBOD, Physics - Cornell University, STEPHANIE LEE, Materials Science and Engineering - Cornell University, BETTINA JOHN, Chemical Engineering - Cornell University, ANGIE WOLFGANG, Physics - Cornell University, CHAKESHA LIDDELL, Materials Science and Engineering - Cornell University, FERNANDO ESCOBEDO, Chemical Engineering - Cornell University, ITAI COHEN, Physics - Cornell University — We report that monolayers of hard peanut-shaped colloidal particles consisting of two connected spherical lobes order into a crystalline phase at high area fractions. In this “lobe- close-packed” (LCP) crystal, the peanut particle lobes occupy triangular lattice sites, much like closed-packed spheres, while the connections between lobe pairs are randomly oriented, uniformly populating the three crystalline directions of the underlying lattice. Using optical microscopy, we directly observe defect nucleation and dynamics in sheared LCP crystals. We find that many particle configurations form obstacles blocking dislocation glide. Consequently, in stark contrast to colloidal monolayers of close-packed spheres, single dislocation pair nucleation is not the only significant energetic barrier to relieving an imposed shear strain. Dislocation propagation beyond such obstructions can proceed only through additional mechanisms such as dislocation reactions. We discuss the implications of such restricted defect mobility for the plasticity of LCP crystals.

8:12AM H39.00002 Elastic Theory of Defects in Toroidal Crystals, LUCA GIOMI, MARK BOWICK, Syracuse University — Crystalline assemblages of identical sub-units packed together and elastically bent in the form of a torus have been found in the past ten years in a variety of systems of surprisingly different nature, such as viral capsids, self-assembled monolayers and carbon nanomaterials. We investigate the structural properties of toroidal crystals and we provide a unified description based on the elastic theory of defects in curved geometries.

8:24AM H39.00003 Hopping Conduction and Bacteria: Transport Properties of Disordered Reaction-Diffusion Systems, ANDREW MISSEL, KARIN DAHMEN, University of Illinois, Urbana-Champaign — Reaction-diffusion (RD) systems are used to model everything from the formation of animal coat patterns to the spread of genes in a population to the seasonal variation of plankton density in the ocean. In all of these problems, disorder plays a large role, but determining its effects on transport properties in RD systems has been a challenge. We present here both analytical and numerical studies of a particular disordered RD system consisting of particles which are allowed to diffuse and compete for resources (2λ → A) with spatially homogeneous rates, reproduce (A → 2A) in certain areas (‘oases’), and die (A → 0) everywhere else (the ‘desert’). In the low oasis density regime, transport is mediated through rare “hopping events” in which a small number of particles diffuse through the desert from one oasis to another; the situation is mathematically analogous to hopping conduction in doped semiconductors, and this analogy, along with some ideas from first passage percolation theory, allows us to make some quantitative predictions about the transport properties of the system on a large scale.

8:36AM H39.00004 Hard Discs on the Hyperbolic Plane, CARL MODES, RANDALL KAMIE, University of Pennsylvania — We examine a simple hard disc fluid with no long range interactions on the two dimensional space of constant negative Gaussian curvature, the hyperbolic plane. This geometry provides a natural mechanism by which global crystalline order is frustrated, allowing us to construct a tractable model of disordered monodisperse hard discs. We extend free area theory and the virial expansion to this regime, deriving the equation of state for the system, and compare its predictions with simulation near an isostatic packing in the curved space.
8:48AM H39.00005 Experimental Observation of Quantized Vortex Reconnection and Turbulence in Superfluid Helium
Matthew PAOLETTI, University of Maryland, KATEPALLI SREENIVASAN, International Centre for Theoretical Physics and University of Maryland, DANIEL LATHROP, University of Maryland — We present experimental studies of the first direct visualization of reconnecting quantum vortices and the decay of superfluid turbulence in $^4$He. Micron-sized solid hydrogen particles are used for particle tracking. The cores of the superfluid vortices trap the hydrogen particles, thereby allowing direct visualization of the dynamics of the line-like defects. We generate superfluid turbulence by driving a thermal counterflow. After pulsing the counterflow, the system relaxes through a cascade of reconnection events. We examine the dynamics of pairs of particles trapped on reconnecting vortices and observe that these particles separate as power laws in time with a scaling exponent distributed about the predicted value of $1/3$. We show that reconnection leads to power-law tails in the velocity probability distribution function, which is in stark contrast to the Gaussian tails that are ubiquitous in classical turbulence and thermal motion.

9:00AM H39.00006 Slippery or sticky boundary conditions: control of wrinkling in metal-capped thin polymer films by selective adhesion to substrates
Hugues VanDeParre, Julien Leopoldes, Christophe Pouillard, Sylvain Desprez, Cyprien Gay, Gwenaelle Derue, Pascal Damman, Laboratoire de Physicochimie des Polymères, Université de Mons-Hainaut Team, Centre de Recherche Paul-Pascal, Université de Bordeaux Collaboration — As demonstrated by countless studies, sheets are more easily bent than stretched. Under planar forces, a thin sheet will thus deform out of plane by forming wrinkles. Surface buckling or wrinkling can be generated in various systems such as rigid thin films supported on elastomers, or gels that could be swollen or dried. Here, we describe an original and simple method to control the spatial layout of wrinkles in polymer/metal bilayer systems. To generate surfaces with a tailor-made buckling pattern, we have tuned the boundary conditions at the polymer-substrate interface using chemically patterned substrates with highly contrasted surface free energies ($\gamma$), easily produced by microcontact printing of alkanethiols on gold substrates. In addition, to explain our original variant of the experiments, we will also expand the existing mechanisms and models described in the literature to take into account the adhesion at the polymer-substrate interface.

9:12AM H39.00007 Shrinky Dinks: Dynamic Shape Transformations
Ajay Gopinathan, Michelle Khine, Arnold Kim, University of California, Merced — Biaxially oriented polystyrene thermoplastic sheets (shrinky dinks) have been recently used by one of us (Khine, Lab on a Chip, 2008) as a template for rapid and non-photolithographic microfluidic pattern generation. This method utilizes the shrinkage properties of the shrinky dinks upon heating to generate microscale structures. During the heating process the sheets show a variety of non-trivial three dimensional intermediate structures before returning to a shrunken flat state upon completion of the process. We show that these structures arise due to the imposition of a non-uniform spatial metric on the sheet which in turn is governed by the dynamic temperature gradients generated in the sheet. Our results allow us to quantitatively describe the dynamic sequence of structures generated and suggest routes to the design and fabrication of different structures in a controlled fashion.

9:24AM H39.00008 The Roll of Friction in the Mechanical Failure Properties of a Polymer Particulate Composite
Donald Wiegand, Brett Reddingius, ARDEC, Picatinny, NJ USA, Kevin Ellis, Claire Leppard, AWE, Aldermaston, U — The mechanical failure properties of a composite containing an organic crystalline particulate and a polymer-plastizer binder have been investigated as a function of hydraulic pressure between 0.1 and 138 MPa. The results indicate that in a low pressure range between about 0.1 and 7.0 MPa crack processes are important in failure. The pressure dependence of the compressive strength is attributed to coulomb friction between surfaces of closed cracks, and from the observed linear increase of the strength with pressure a friction coefficient is obtained. Friction coefficients can also be obtained from the ratio of compressive to tensile strength and in addition from the angle which the failure plane makes with the direction of the applied stress. Both at 0.1 MPa and 138 MPa friction coefficients were obtained from these three separate observations in agreement and this is taken as strong evidence for the importance of this friction in determining strength and mechanical failure for this composite.

9:36AM H39.00009 Force-driven transport in entropy barriers
Kevor Kevorkian, Nabil Laachi, Martin Kenward, University of Minnesota, Ehud Yariv, Technion — We consider theoretically the transport of a point-sized Brownian particle in a two-dimensional channel with a slowly varying, periodic cross-section. Such channels are associated with the concept of an “entropy barrier,” where the change in the number of available states for a system depends on the transport through the channel. Using generalised Taylor-Aris dispersion theory and long-wavelength asymptotics, we exactly compute the mean particle velocity and effective diffusivity (dispersivity) for two cases: electrohydroptic transport in an insulating channel and motion under the influence of a constant force. At the same time, we arrive at rational definitions for the concept of an entropy barrier as a function of the driving force. The agreement between simulations and the exact calculation for a constant force is excellent and represents a significant advance over existing models of the transport process.

9:48AM H39.00010 Friction and wear of nanocrystalline diamond coatings
Abhishek Kothari, Brian Sheldon, Brown University, Xingcheng Xiao, GM research, Kyung-Suk Kim, Brown University, Leo Levy, GM — Nanocrystalline diamond films were tested for friction and wear response using a pin on disc tribometer. COF, starting with 0.7 successively drops to 0.1 as the wear progresses. Understanding this friction and wear response is important to minimize wear of these materials as tool coatings. SEM images at the periphery of wear tracks indicate the presence of ring cracks which are due to stress at the circle of contact exceeding the tensile strength. Effects of engineering the stress on the wear have been verified experimentally. Estimation of wear rate in these coatings is of high importance. AFM was used to obtain topography information on wear tracks of the film successively after 2K-200K pin revolutions in the tribometer. It is noted that peak heights of the asperities were decreasing with wear. Image analysis of the topographical evolution of the successive wear tracks could provide an estimation of the wear rate. This analysis also indicates that the distribution ofasperity contact size shifts towards larger size with successive wear of the film. Previous studies of Krim, Hurtado and Kim revealed that the frictional stresses of individual asperities are dependent on theasperity contact sizes — the larger the asperity contact size, the lower the frictional stresses. The micromechanics model ofasperity friction explains well the decreasing coefficient of friction with progression of wear.

10:00AM H39.00011 Ultra-high vacuum cryotribology of diamond and diamond-like films
Matthew Aggleton, P. Taborek, University of California, Irvine — We have used a sliding block tribometer (described in J.C. Burton, P. Taborek, and J.E. Rutledge, TRIBOLOGY LETTERS 23, 131, 2006) to measure the temperature dependence of the kinetic friction coefficient of single crystal diamond on various types of CVD diamond films including microcrystalline diamond, nanocrystalline diamond, and diamond-like carbon. We have also studied various other solid and fluid lubricants. These measurements have been performed in ultra-high vacuum and at temperatures ranging from 6 to 300 Kelvin. Although microcrystalline diamond has a low friction coefficient in air, in vacuum, the friction coefficient rises to approximately 0.7 and is independent of temperature. Nanocrystalline diamond is a much better tribological material in vacuum, particularly for T $>$ 240K. Near 240K there is a reversible transition to a higher friction state. We will discuss the correlation between the tribological properties and the material properties such as sp2/sp3 ratio, hydrogen content, and grain size. This work is supported by Extreme Friction: MURI AFOSR # FA9550-04-1-0381.
10:12AM H39.00012 Quartz Crystal Microbalance Studies of Temperature Rise in a Sliding Contact, JACQUELINE KRIM, BENJAMIN DAWSON, MATTHEW WALKER, CHERNO JAYE, DOUGLAS IRVING, DONALD BRENNER, North Carolina State University — The exact relation between temperature rise in a sliding contact and frictional energy dissipation is of great technological importance, but poorly understood at a fundamental level. Temperature rise is presumably due to frictional heating that results from phononic and electronic excitations, but efforts to relate temperature rise to friction and sliding velocity have proven very difficult. We have performed QCM studies of adsorbed Krypton monolayers, and also joint QCM-STM studies, to examine temperature rise associated with friction in two well characterized geometries. In the first, we utilized the static phase diagram of two-dimensional Kr adsorbed on graphite as compared to the dynamic phase diagram (with the Kr layer sliding) to determine temperature rise. In the second study, we have recorded frequency shift data for a QCM with indium electrodes in contact with an STM tip while increasing the sliding speed to a point where melting is indicated. A temperature rise on the order of 10 (40-100) degrees is observed in the first (second) geometry. Comparisons to theory yield plausible fit parameters.

1Work supported by NSF and AFOSR
2Present Address: Brookhaven Nat.Lab.

10:24AM H39.00013 Combined ab initio and classical molecular dynamics simulations of the tribological properties of rare gas monolayers sliding on metal surfaces, MARIA CLELIA RIGHI, CNR-INFM S3 National Research Center, Via Campi 213/a Modena, Italy, MAURO FERRARIO, Universita' di Modena e Reggio Emilia — Progress in the ability of understanding tribological properties in adsorbed film systems is of paramount importance to unravel fundamental issues in the emerging field of nanoscale science and technology. Many extensive studies have used a quartz-crystal microbalance (QCM) to measure the friction between adsorbed rare gas monolayers and metal substrates. In this work, we report a theoretical investigation of the tribological behavior of different rare gas-metal adsorbate systems, namely, Ar, Kr, Xe on Cu(111), and Xe on Ag(111), based on combined ab initio and classical molecular dynamics simulations. The frictional properties are analyzed in details as a function of system temperature, presence of interlayer defects, and load. The numerical simulations suggest that the simultaneous presence of thermal effects and of interlayer defects, lowering significantly the activation energy barrier, causes a considerable reduction of the static friction threshold. An unexpected dependence on load is also predicted. In particular, we show that friction of anticorrupting systems can be dramatically decreased by applying an external load [1]. The counterintuitive behavior that deviates from the macroscopic Amonton law is dictated by quantum mechanical effects that induce a transformation from anticorruption to corrugation in the near-surface region. [1] M. C. Righi and M. Ferrario, Phys. Rev. Lett. 99, 176101 (2007).

10:36AM H39.00014 Solid-fluid transitions at high sliding rates at Al/Al interfaces, J.E. HAMMERBERG, B.L. HOLIAN, Los Alamos National Laboratory, R. RAVELO, University of Texas, El Paso, T.C. GERMANN, Los Alamos National Laboratory — Large scale NonEquilibrium Molecular Dynamics (NEMD) simulations (1.4 \times 10^6 \text{ atoms}) for single crystal Al have shown a transition as a function of sliding velocity from a defective solid phase to a fluid phase beyond a critical velocity, \( v_c \), which depends very nearly linearly with the homologous temperature \( T/T_m \), where \( T_m \) is the melting temperature and \( T \) is the sample temperature far from the interface. Above \( v_c \), a Couette flow pattern develops with a slope which is independent of velocity. We discuss the properties of this transition and the power law dependence of the frictional force with velocity observed in this regime.

This work was supported by the U.S. Department of Energy under contract DE-AC52-06NA25396

10:48AM H39.00015 ABSTRACT HAS BEEN MOVED TO SESSION H8 –

Tuesday, March 11, 2008 8:00AM - 10:24AM –
Session H40 DMP DCOMP: Focus Session: Earth and Planetary Materials I Morial Convention Center 232

8:00AM H40.00001 Elasticity of (Mg,Fe)O through the spin transition of iron in the lower mantle, JONATHAN CROWHURST, Lawrence Livermore National Laboratory — Recently, the important question of spin-pairing transitions of iron from high-spin (HS) to low-spin (LS) states in ferropericlase (Ref. 1 and references therein) affecting the lower mantle’s density and seismic-wave velocities has been recognized (2,3). Since knowledge of this deep and inaccessible region is derived largely from seismic data, it is essential to determine the influence of the spin transition on elastic wave velocities at lower-mantle pressures. We here discuss the results of measurements of the elastic tensor of (Mg,9.4Fe0.6)O up to 60 GPa using impulsive stimulated light scattering. We find that all tensor elements soften substantially through the HS to LS transition, and that the softening occurs over an extended pressure range from 40 GPa to at least 60 GPa at room temperature. By invoking a simple thermodynamic description (4) of the transition we can compare our results to literature compression data (2,5) obtained from material with the higher iron concentrations likely to be found in ferropericlase in the lower mantle. The agreement is good and thus suggests that the thermodynamic description is reasonable. This in turn allows us to predict the effect of high temperature on the transition; we find that as temperature is increased the transition region is extended (see also Ref. 6) and the magnitude of the softening decreases. We conclude that although the spin transition in (Mg,Fe)O is too broad to produce an abrupt seismic discontinuity in the lower mantle, the transition will produce a correlated negative anomaly for both compressional and shear velocities that extends throughout most if not all of the lower mantle.


This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

8:36AM H40.00002 Elasticity of ferropericlase at Earth’s lower mantle conditions, RENATA WENTZCOVITCH, JOAO JUSTO, ZHONGQING WU, CESAR DA SILVA, U of Minnesota — The thermoelastic properties of ferropericlase Mg1-xFe xO (x = 0.1875) across the iron high-to-low spin crossover at lower mantle conditions have been investigated by combining first principles calculations with a thermodynamics model of this system. At room temperature the transition is somewhat sharp and the effect on the bulk modulus is quite dramatic. Along a typical geotherm the transition should occur across most of the lower mantle with a noticeable bulk modulus reduction in the mid lower mantle. This transition should also alter noticeably the magnitude of velocity heterogeneities caused by lateral temperature changes.

1Research supported by NSF/EAR NSF/IITR and ITAMIT
8:48AM H40.00003 Inter-site Partitioning of Iron in Wadsleyite at High Pressures. ROSE PEREA, BORIS KIEFER, Department of Physics, New Mexico State University — (Mg1-x,Fex)2SiO4 — wadsleyite is thought to be the most abundant metal in the upper part of the Earth’s transition zone (410 -520 km depth). Wadsleyite contains three crystallographically non-equivalent octahedral sites, M1, M2, and M3. Experimentally, it has been observed that the M2 site is depleted in iron relative to the M1 and M3 sites. This asymmetric partitioning may affect the melting temperature and the density of iron bearing wadsleyite and influence the transport of mass, momentum, and energy across the transition zone. We performed LDA and GGA first-principle calculations of ferrous iron substitutions in the three crystallographically distinct octahedral sites: M1, M2, and M3. At low pressures, we find that the pressure sensitivities of the iron occupancies are consistent with the experimental observations that the M2 site is depleted in iron and independent of the magnetic moment of iron. This finding indicates that the inter-octahedral site partitioning of iron is due to the presence of the d-orbitals. If this finding can be corroborated our results will affect the understanding of the partitioning of other divalent transition metals and geochemical trace elements in wadsleyite, the most abundant mineral in the upper part of the Earth’s transition zone.

9:00AM H40.00004 First principles studies on several major phase transitions in Earth upper mantle. YONGGANG YU, Univ. of Minnesota, ZHONGQING WU, U of Minnesota, RENATA WENTZCOVITCH, U of Minnesota, CHEMICAL ENGINEERING AND MATERIALS SCIENCE TEAM — First principles quasi-harmonic free energy calculations have been conducted to study several important phase transitions in mantle minerals with compositions Mg2SiO4 and MgSiO3 under realistic Earth’s mantle conditions. We find encouraging and similar level of agreement with experiments for thermodynamic and vibrational properties and phase transition boundaries in all cases where comparisons between results and data are possible. We also find systematic trends: 1) equations of state and thermodynamic properties of single crystalline phases are best described by the LDA; 2) phase boundaries are bracketed by LDA and GGA results, with GGA offering the upper bound transition pressure and being somewhat closer to the experimental ones. A summary of these results is offered for forsterite, wadsleite, ringwoodite, periclase, perovskite, post-perovskite, low clin-, and high clin-enstatite, and garnet, as well as phase transitions between them. In overall these results can supplement high-PT experimental data on these minerals. (Research supported by NSF/EAR 013533, 0230319, 0635990, and NSF/ITR 0428774 (VLab), and Minnesota Supercomputing Institute.)

9:12AM H40.00005 The Phase Diagram of Portlandite, Ca(OH)2 at Pressures up to 40 GPa. BORIS KIEFER, MEGAN LOCKWOOD, Department of Physics; New Mexico State University — Hydroxides have attracted significant scientific interest over the past decades. They have been used as analogues to further our understanding of hydrogen bonding in complex materials. Several experimental observations suggest that portlandite undergoes reversible solid state amorphization at high pressures but the cause for this transition and its appearance in portlandite remains unknown. We performed static (0 K) first-principle calculations based on the GGA within the framework of Density-Functional-Theory in order to explain the phase diagram of portlandite for pressures up to 40 GPa. All structures were fully relaxed to determine the ground state energy. We find that a split-site model for the hydrogen array is energetically preferred consistent with neutron diffraction experiments. At a pressure of ~4.5 GPa we observe a phase transition from trigonal to monoclinic symmetry in agreement with previous studies. At all higher pressures we find that the monoclinic structure is the ground state of portlandite. However, we identified several energetically comparable structures. This indicates that the potential energy surface of portlandite has a surprisingly complex structure. The interplay of these structures suggest that the solid state amorphization is driven by non-hydrostatic stress and allows to rationalize experimentally observed differences between portlandite powders and single-crystals.

9:24AM H40.00006 High PT elasticity within the quasiharmonic approximation with relaxed thermal stresses. PIERRE CARRIER, JOAO F. JUSTO, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, 55455. — We describe in detail a method to compute high PT elasticity within the quasiharmonic approximation (QHA). This approach differs from the usual formulation used to compute the statically constrained high PT elastic constants by including corrections due to deviatoric thermal stresses. The formulation is general and valid for crystals with up to triclinic symmetry. We use perovskite and post-perovskite phases of MgSiO3 to exemplify the use of the method to calculate elasticity and crystal structures at high PT.

9:36AM H40.00007 Quantum Monte Carlo Study of Elastic Instability in Stishovite. K.P. DRIVER, Ohio State, R.E. COHEN, Carnegie Institution of Washington, P.L. RIOS, M.D. TOWLER, R.J. NEEDS, Cambridge, J.W. WILKINS, Ohio State — Stishovite is an octahedrally coordinated polymorph of silica which is stable at pressures within Earth’s lower mantle (10 GPa). Elastic properties of stishovite are important for explaining seismic structure and it serves as a model system for other six-coordinated silicates. Near 50 GPa, stishovite transforms to the CaCl2-type structure due to an instability in the elastic shear modulus. The instability was first predicted by density functional theory (DFT) calculations and later confirmed by Raman spectroscopy and X-ray diffraction. Quantum Monte Carlo accurately predicts elastic constants and benchmarks previous DFT results on the stishovite elastic instability. Over the pressure range of 0 to 50 GPa, QMC shows the elastic shear modulus softens from 270 to 0 GPa in agreement with previous DFT and experimental results. Computations were performed at NERSC. Funding provided by the NSF (EAR-0530282, EAR-0310139) and the DOE (DE-FG02-99ER45795).

9:48AM H40.00008 Pressure dependence of lattice anharmonicity and phonon lifetime in MgO: a first-principles calculation and implications for lattice thermal conductivity. XIAOLI TANG, JIANJUN DONG, Auburn University — We report a recent first principles calculation of harmonic and anharmonic lattice dynamics of MgO. The 2nd order harmonic and 3rd order anharmonic interatomic interaction terms are computed explicitly, and their pressure dependences are discussed. The phonon mode Grüneisen parameters derived based on our calculated 3rd lattice anharmonicity are in good agreement with those estimated using the finite difference method. The phonon lifetime due to lattice anharmonicity is calculated based on the single mode excitation approximation (SMEA). We have further estimated the isotope effect on phonon lifetime within the random mass disorder approximation. The implications for lattice thermal conductivity at high pressure are discussed based on a simple kinetic transport theory.
from carbon-arc produced soot allowed the growth and characterization of both bulk and thin-film samples. Crystalline C
structure invites special attention and continues to stimulate animated speculation. The availability in 1990 of macroscopic amounts of purified C
unquestionably an arrestingly beautiful molecule. The high symmetry of the 12 pentagonal and 20 hexagonal faces symmetrically arrayed in a soccer-ball
structure?

10:12AM H40.00010 First-principles study of MgSiO₃ at core-mantle boundary conditions.
SIU-CHUNG SUNG, The Chinese University of Hong Kong; JONES TSZ-KAI WAN — Perovskite MgSiO₃, is an important mineral in geoscience studies. It
plays a crucial role in the understanding of geophysical and geochemical activities taken place in the Earth’s interior. In this talk, we report our recent work on
First-principles molecular dynamics (FPMD) simulations of solid MgSiO₃ perovskite and post-perovskite, and molten MgSiO₃ at core-mantle boundary (CMB)
conditions. The equations of state are determined at pressures up to 200 GPa and temperatures up to 6000K. The post-perovskite phase is found to be favoured
over the perovskite at pressures above 102 GPa at zero temperature. Melting of MgSiO₃ has been observed by heating both perovskite and post-perovskite at high
temperatures (≥6000 K). The melting curve and electronic structures of solid and molten MgSiO₃ are also presented. Our simulated results thus provide
useful constraints on structure and phase stability of MgSiO₃, which is the key to the understanding of deep-earth phenomena, such as the D''' discontinuity and
seismic anisotropies in D'' layer. More importantly, the phase transformation of MgSiO₃ studied in this work provides insights into other aspects of geosciences
like chemical heterogeneity and mantle convection, which may lead to a better model of the Earth’s evolution.

11:15AM J1.00001 Oliver E. Buckley Prize Talk: Why are we so excited about carbon nanostructures?
MILDRED DRESSELHAUS, MIT — There is much current excitement about the interesting new physics and unusual physical properties of carbon nanostructures, particularly carbon nanotubes and graphene. A brief review will be given of the physical underpinnings of carbon nanostructures that were developed over the past 60 years, starting with the electronic structure and physical properties of graphene and graphite, and then moving to graphene intercalation compounds which contained the first carbon nanostructures to be studied experimentally. Liquid carbon studies were precursors to the fullerene family of nanostructures and vapor grown carbon fibers were precursors to carbon nanotubes. Particular emphasis is given to the recent developments in our understanding of the photophysics of carbon nanotubes and graphene, with perspectives on future research directions for these fields.

JULIA PHILLIPS, Sandia National Laboratories — Securing a viable, carbon neutral energy future for humankind will require an effort of gargantuan proportions. As outlined clearly in a series of workshops sponsored by the DOE Office of Basic Energy Sciences (http://www.sc.doe.gov/bes/reports/list.html), fundamental advances in scientific understanding are needed to broadly implement many of the technologies that are held out as promising options to meet future energy needs. Technologies of interest range from solar energy, to nuclear energy, to approaches to clean combustion. Using solid state lighting based on inorganic materials as an example, I will discuss some recent results and new directions, emphasizing the multidisciplinary, team nature of the endeavor. I will also offer some thoughts about how to encourage translation of the science into attractive, widely available products – a significant challenge that cannot be ignored. This case study offers insight into approaches that are likely to be beneficial for addressing other aspects of the energy security challenge.

12:27PM J1.00003 James C. McGroddy Prize Talk: Superconductivity in alkali-metal doped Carbon-60
ARTHUR HEUBARD, University of Florida — Carbon sixty (C₆₀), which was first identified in 1985 in laser desorption experiments, is unquestionably an arresting beautiful molecule. The high symmetry of the 12 pentagonal and 20 hexagonal faces symmetrically arrayed in a soccer-ball-like structure invites special attention and continues to stimulate animated speculation. The availability in 1990 of macroscopic amounts of purified C₆₀ derived from carbon-arc produced soot allowed the growth and characterization of both bulk and thin-film samples. Crystalline C₆₀ is a molecular solid held together by weak van der Waals forces. The fcc structure has a 74% packing fraction thus allowing ample opportunity (26% available volume) for the intercalation of foreign atoms into the interstitial spaces of the three dimensional host. This opportunity catalyzed much of the collaborative work amongst chemists, physicists and materials scientists at Bell Laboratories, and resulted in the discovery of superconductivity in alkali-metal doped C₆₀ with transition temperatures (T_c) in the mid-30-kelvin range. In this talk I will review how the successes of this initial team effort stimulated a worldwide collaboration between experimentalists and theorists to understand the promise and potential of an entirely new class of superconductors containing only two elements, carbon and an intercalated alkali metal. Although the cuprates still hold the record for the highest T_c, there are still open scientific questions about the mechanism that gives rise to such unexpectedly high T_c's in the non-oxide carbon-based superconductors. The doped fulleranes have unusual attributes (e.g., narrow electronic bands, high disorder, anomalous energy scales, and a tantalizing proximity to a metal-insulator Mott transition), which challenge conventional thinking and at the same time provide useful insights into new directions for finding even higher T_c materials. The final chapter of the 'soot to superconductivity' story has yet to be written.

1:03PM J1.00004 James C. McGroddy Prize Talk: What Was New About C60
ROBERT HADDON, University of California at Riverside — C₆₀ was named molecule of the year by Science in 1991, and in this talk I will discuss what I consider to be the most novel features of the molecule. In some ways C₆₀ is truly unique and the discovery of the molecule in 1985 and its subsequent synthesis in 1990 blazed a trail of new chemical and physical properties that is unlikely to be surpassed by any other molecule. I will discuss the electronic structure of C₆₀, its magnetism, and the conductivity and superconductivity shown by the alkali metal-doped phases.

1 Acknowledgement to the ESF program “Mineralogy and Chemistry of Earth’s core (MCEC)”, Swedish Research Council (VR), Swedish Foundation for Strategic Research (SSF), Swedish National Infrastructure for Computing (SNIC), Deutsche Forschungsgemeinschaft

1 Work Performed at AT&T Bell Laboratories.

12:27PM J2.00003 Condensed Matter Theory: From Models to First Principles1, MARVIN COHEN, University of California, Berkeley — It can be argued that modern condensed matter theory (CMT) started 100 years ago. Models of materials explained many solid state phenomena and properties. However, only in the past 50 years—during the “PRL Era”—can it be argued that a significant number of ab initio calculations for real materials have been done. After some historical comments, the primary conceptual models will be described. This discussion will be followed by examples of current theoretical work on explaining and predicting properties and phenomena associated with “real materials.”

1This work was supported by National Science Foundation Grant No. DMR07-05941, and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

1:03PM J2.00004 NMR and the BCS Theory, CHARLES P. SLICHTER, University of Illinois at Urbana-Champaign — The talk will review the status of superconductivity research in the early 1950s, Bardeen’s thoughts about the role of an energy gap in producing superconductivity, our ideas that NMR experiments might test his ideas, and about the experimental challenge my student Chuck Hebel and I had to overcome: How can one do NMR in a perfect diamagnet (which therefore excludes magnetic fields!), the surprising results we found, then the arrival of the theory of Bardeen, Cooper, and Schrieffer, and how applying their theory to relate NMR to ultrasonic absorption verifies the essential idea of the theory (their wave function of electron pairs).


Tuesday, March 11, 2008 11:15AM - 2:15PM — Session J3 DCMP: Kondo Screening and Quantum Criticality from the Spatial Limit: From Single Spins to Droplets to Lattices Morial Convention Center RO2 - RO3

11:15AM J3.00001 How does a Kondo impurity respond to its local environment?1, ANDREAS HEINRICH, IBM Research — The interplay between localized electrons on a magnetic atom and the conducting electrons in a metal can lead to intriguing many-body ground states such as the Kondo effect. When a spin is Kondo screened by conduction electrons the entire spin system performs a complicated dance that results in the formation of a spin singlet at sufficiently low temperature. For simplicity, most theoretical considerations of Kondo screening focus on magnetic impurities with the lowest possible spin $S = 1/2$. Such systems can be studied experimentally in exquisite detail and with great control using quantum dots in semiconductor heterostructures or carbon nanotubes. However, in Kondo systems consisting of localized magnetic atoms, the spin is often larger, making the Kondo effect richer and more complex. Here we use the imaging and spectroscopy capabilities of a scanning tunnelling microscope to study how the Kondo screening of a known high-spin atom is determined by its local environment. Co and Ti atoms were deposited on a thin insulating layer ($Cu_2$) on a copper substrate. We study the influence of external magnetic fields, crystalline magnetic anisotropy, as well as spin-coupling to surrounding atomic spins on the Kondo effect that forms on the Co or Ti atoms. We find that the anisotropy of the crystalline field quenches the high-spin system of Co ($S = 3/2$) into an effective $S = 1/2$ Kramers doublet. Surprisingly, much of the impact of these environmental factors on the complex many-body ground state can be understood simply through their effects on the energy levels of the unscreened spin.

1This work was done in collaboration with A.F. Otte, C.F. Hirjibehedin, H. Brune, M. Ternes, and C.P. Lutz.
11:51AM J3.00002 Geometric Manipulation of Quantum Phase and Correlations in Nanoassembled Spin Systems*1, HARI C. MANOHARAN, Department of Physics, Stanford University — The single-impurity Kondo problem, in which an isolated magnetic impurity in a non-magnetic metallic host has its spin screened by spins of conduction electrons, has been extensively studied both theoretically and through bulk experiments. Recently new methods have allowed detailed experimental probing of the prototype single-impurity Kondo effect of individual magnetic atoms. In addition, spin interactions with confined electron states were used to materialize “quantum mirages” consisting of a nonlocal single-impurity Kondo effect. When many spin and spatial states are present in a bulk conductor or on its surface, the interactions between them may engender novel collective effects. Using a scanning tunneling microscope we assembled and studied atomically precise arrangements of (magnetic) Co atoms and (non-magnetic) CO molecules on the Cu(111) surface. The spin degeneracy of single magnetic atoms and the conduction electrons alone provide necessary ingredients for Kondo physics. When combined with quantum resonators, Kondo phase shifts can be measured by using the nanostructures as quantum interferometers. We study the effects of adding to the degeneracy of the system in two controlled ways: engineering degeneracies in the spatial states of confined electrons coupled to the spins, and engineering lattices of many spins coherently coupled through electrons. The first type of experiment has enabled a novel method to read out and geometrically manipulate the quantum phase associated with state superpositions. The second class of experiments has enabled investigation of the finite size spin physics of Kondo droplets. In these periodic structures we observe signs of quantum interference and spin correlation effects when the geometries are suitable tuned relative to the Fermi wavelength of the host electron systems. These new quantum materials act as model systems for understanding complementary physics in complex matter.

*This work was done in collaboration with L. S. Mattos, C. R. Moon, B. K. Foster, G. Zeltzer, and C. P. Lutz.

12:27PM J3.00003 Kondo Physics at the Nanoscale*1, DIRK MORR, University of Illinois at Chicago — Recent experimental advances have made it possible to study the Kondo effect in nanoscale structures. These achievements are of great importance because they do not only allow us to manipulate the Kondo screening of single magnetic impurities, but also provide us with the unique opportunity to study how Kondo screening and coherence evolve on different length-scales from a single Kondo impurity to the Kondo lattice. In this talk, I present two examples of novel Kondo physics emerging in nanostructures. First, I demonstrate that the presence of electronic eigenmodes in a nanostructure gives rise to unconventional properties of a Kondo screened magnetic impurity [1]. In particular, the Kondo temperature, $T_K$, of a magnetic impurity located inside the nanostructure varies with the impurity’s location and is determined by the eigenmodes’ spatial structure. Moreover, the modes’ frequency dependence leads to a linear relation between $T_K$ and the local density of states, in stark contrast to the conventional Kondo effect. Second, I discuss Kondo screening and the onset of coherence in finite size Kondo lattices, so-called Kondo droplets. I show that in such Kondo nanostructures, the hybridization and the coherent coupling of the Kondo resonances can be resonantly enhanced or suppressed via changes in the droplet’s geometry and lattice constant. Moreover, I demonstrate how these properties of the Kondo droplet evolve with increasing droplet size. Finally, I discuss how the ability to manipulate the properties of Kondo droplets might provide novel insight into the origin of quantum criticality, which is a central point in understanding the unconventional non-Fermi liquid properties of Kondo lattice systems, such as the heavy-fermion materials.

*Supported by EPSRC (UK) GR/S20567/0.


1:39PM J3.00005 Quantum Criticality in 3He bi-layers, CATHERINE PEPIN, SPHT, CEA-Saclay — No abstract available.


11:15AM J4.00001 Scientists in an alternative vision of a globalized world*1, AYSE ERZAN, Department of Physics, Istanbul Technical University, Maslak, Istanbul — Why should “increasing the visibility of scientists in emergent countries” be of interest? Can increasing the relevance and connectedness of scientific output, both to technological applications at home and cutting edge basic research abroad contribute to the general welfare in such countries? For this to happen, governments, inter-governmental and non-governmental organizations must provide incentives for the local industry to help fund and actively engage in the creation of new technologies, rather than settling for the solution of well understood engineering problems under the rubric of collaboration between scientists and industry. However, the trajectory of the highly industrialized countries cannot be retraced. Globalization facilitates closer interaction and collaboration between scientists but also deepens the contrasts between the center and the periphery, both world wide and within national borders; as it is understood today, it can lead to the redundancy of local technology oriented research, as the idea of a “local industry” is rapidly made obsolete. Scientists from all over the world are sucked into the vortex as both the economic and the cultural world increasingly revolve around a single axis. The challenge is to redefine our terms of reference under these rapidly changing boundary conditions and help bring human needs, human security and human happiness to the fore in elaborating and forging alternative visions of a globalized world. Both natural scientists and social scientists will be indispensable in such an endeavor.

*Partial support from the Turkish Academy of Sciences is gratefully acknowledged.
11:45 AM J4.00002 Globalizing Science and Engineering, VENKATESH NARAYANAMURTI, Harvard University — In this talk I will review recent trends in Science and Engineering Research and Education in an increasingly interconnected, “flat” world. The enormous economic transformation being fueled by technology will, over a period of time, lead to new models of interaction among universities, industry and governments. Scientists and Engineers in “emergent” countries may be expected to play a key role in this “new” world order.

12:15 PM J4.00003 The Mutual Benefit of International Research Interactions, MONICA OLVERA DE LA CRUZ, Northwestern University — Emergent economies provide a fruitful source of scientific knowledge. We have the responsibility to nurture interactions to increase scientific knowledge in the world. Moreover, we have benefited greatly from discoveries and education provided to scientists and engineers in emergent economies. I will give examples of successful modes of interactions between the US and emergent economies, and in particular with Latin American countries. I will review the impact of our interactions in their countries and in ours, and ways to increase the impact.

12:45 PM J4.00004 The Invisible Scientist in India – a case study for emergent countries, ANITA MEHTA, S D Bose National Centre — Emergent countries such as India, China, and Brazil, face unique problems in the realisation of their science and technology potential. I will discuss the situation in India, which may be relevant at least in part to the others. The basic focus of the talk will be the possible ways in which the invisible scientist, the person on the ground who has no part in the pyramid of the science establishment, can be rendered more visible both for her or his own sake, and to prevent the erosion of an enormous intellectual potential by a still continuing brain drain.

1:15 PM J4.00005 Panel Discussion —

Tuesday, March 11, 2008 11:15AM - 1:39PM —
Session J5 CSWP FGSA: Where is the Center of Mass for Family, Career, and Self? Morial Convention Center R01

11:15 AM J5.00001 Career Planning in Harmony with Family Values and Needs, ARCHANA DUBEY, UCF — Balancing career and family! Balancing what you love and who you love!! It is such an attention getting topic. And yet, if you really think about it, people have been doing it for ages. What makes it challenging in today’s world is the dual income families that throw off-balance of traditional style of balancing family and profession. Balancing family and career is not as difficult. The question is more meaningful when you ask how do you find the right balance, and in fact, what is the right balance? How do you know you are there? Happiness at home and self esteem due to work is genderless issue however, it is essentially talked more in the context of women. Some of the things that could be helpful in achieving the right balance, are time management, proper prioritization, asking for help, a caring family, friends, and most importantly colleagues. In the portfolio of professional passions, it is important to identify the areas that are conducive to possibilities of changing family needs, international families, spouse’s career and job relocation, etc. So, the bottom line question is whether it is possible to find a right balance between family and career? I would submit to you that with passion, courage, open-mindedness, and proper career planning, it is definitely possible. We just need to utilize the same techniques in choosing and sustaining the right balance that we use in identifying research topics and executing it. This discussion will look into further details of the challenges of balancing family and career from the perspective of also an immigrant, and possible ways of overcoming them.

11:51 AM J5.00002 Faculty Work-Family Issues: Finding the Balance at a Liberal Arts College, SUZANNE AMADOR KANE, Physics Department, Haverford College — The demands and expectations on science faculty at liberal arts colleges are in many ways distinct from those at research universities. While these differences can work in favor of easing work-family conflicts, there are also unique problems that faculty can confront in a setting of smaller departments and undergraduate-only institutions. I will discuss how these issues play out for junior and senior faculty, with an emphasis on how concrete policy changes can make the workplace a more family-friendly and supportive environment for all faculty, as well as making liberal arts colleges more attractive options for those seeking physics faculty jobs.

12:27 PM J5.00003 The eye of the storm: Balancing my storm of family, career and self, K. RENEE HORTON, University of Alabama — In knowing that the path I travel is not the usual path traveled by most; this has turned out to be the best path for me and my family. It is very important to prioritize what is important to you and then define the best path for you versus choosing a path and the path chooses your priorities. Coming from a loving and supportive middle class upbringing created a deep sense of family and the importance of family. Early in my life I was determined to have children and a career. Over the last ten years there have been several obstacles to overcome in my storm, but with careful planning, due diligence, and a support system to help maintain calm at the center of my storm I have been able to achieve my goals of pursuing my Doctorate. A complete research plan was put into place into choosing the institution that I would further my academic endeavors in the same manner in which my dissertation research topic has been defined. Just as any successful business, all persons involved in my future success were consulted with equal input into the new endeavor with the full understanding of what this new plan entailed. We decided on the University of Alabama for several reasons: location, weather, flexibility, policies, research and my ability to make a change in the face of science. According to my advisor, I will do that in about two and half years at my graduation ceremony when I become the first African American to receive a PhD in Material Science from the University of Alabama.

1:03 PM J5.00004 Balancing academic career and children: a personal perspective, NINA MARKOVIC, Johns Hopkins University — For women in academia, the tenure review and the desire to have children often happen around the same time. How does one cope with the challenges of an academic career while raising small children? From a personal perspective of an assistant professor and a mother, I will discuss the great challenge of efficient time management and the practical strategies to deal with it.

Tuesday, March 11, 2008 11:15AM - 2:15PM —
Session J6 DCOMP: Effective Potentials and Force Fields for Simulating Biological Macro-molecules Morial Convention Center R04
11:15AM J6.00001 Artifact or reality? Force field issues in the simulation proteins and nucleic acids\(^1\), THOMAS CHEATHAM, University of Utah — Access to ever-increasing computational power is providing the means to critically evaluate the performance of atomistic force fields of biomolecules. With greater sampling, and more detailed comparisons to experiment, limitations and artifacts in the applied simulation protocols and force fields can be discovered and ultimately overcome. Additionally, we are able to more carefully validate and assess the performance of the simulations in comparison with experiment. In this talk, we will outline our experiences in large-scale simulations of protein and nucleic acid systems in the context of the AMBER biomolecular simulation program. Issues related to salt and dihedral parameters will be highlighted in applications ranging from ligand-induced remodeling of dihydrofolate reductase and cytochrome P450 2B4 protein structures to large-scale decoy sets and NMR comparisons of various RNA structures.

\(^1\)Computer time from NSF LRAC MCA0115027 and U. Utah CHPC is greatly acknowledged.

11:51AM J6.00002 Development of a polarizable force field based on the classical Drude oscillator\(^1\), ALEXANDER MACKERELL, Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland — Empirical force field development requires a systematic approach allowing for the development of a practical potential energy function and optimization of physically realistic parameters that reproduce a range of target data. Ongoing efforts in our laboratory include the development of a polarizable force field based on the classical Drude oscillator for a range of molecules representative of biological systems. A central theme in these efforts is the accurate treatment of both atomic interactions as well as condensed phase properties. To achieve this goal extensions of the energy function have been implemented and parameter optimization has been performed targeting a variety of quantum mechanical results and experimental condensed phase properties. An overview of these studies will be presented.

\(^1\)Financial support from the NIH (GM051501 and GM072558) is acknowledged.

12:27PM J6.00003 The AGBNP implicit solvent model: recent advances and applications to biological macromolecules\(^1\), EMILIO GALLICCHIO, BioMaPS Institute, Rutgers University — The Analytical Generalized Born plus Non-Polar (AGBNP) model is an analytical implicit water model suitable for molecular dynamics simulations of small molecules and macromolecules. It is based on an analytical pairwise descreening implementation of the continuum dielectric Generalized Born (GB) model and a non-polar hydration free energy model. AGBNP computes the descreening scaling factors that account for atomic overlaps from the geometry of the solute rather than treating them as geometry-independent parameters fit to numerical or experimental data. The non-polar hydration free energy model is decomposed into a cavity component based on the solute surface area and a solute-solvent van der Waals dispersion energy estimator. The goal of the model is to achieve atomic-resolution accuracy for modelling the many biological systems in which global conformational features are regulated by small and localized control elements. Since its introduction AGBNP has been employed to study a variety of biological problems ranging from peptide conformational propensity and folding, protein allostery, conformational equilibria of protein-ligand complexes, binding affinity prediction, and, more recently, to intrinsically disordered proteins, protein aggregation, the design of virus vaccine carriers, and macromolecular X-ray structure refinement. Recent development work has focused on computational performance enhancements and on improving the accuracy of the model with respect to explicit solvent simulation results. By comparing the details of the solvent potentials of mean force of several peptides calculated with explicit and implicit solvation, we have identified some aspects of the AGBNP model in need of improvement. We are exploring several strategies to address them including the adoption of a molecular surface description of the solute volume, the modelling of high-occupancy hydration sites, and the optimization of the non-polar free energy model.

1:03PM J6.00004 Atomic-level simulations of biomolecular systems with a modified Amber force field\(^1\), CARLOS L. SIMMERLING, Stony Brook University — Experimental methods have been highly successful in determining 3-dimensional biomolecular structures. However, most approaches provide only time- or ensemble-averaged data, making it much more difficult to study the dynamic and energetic aspects of biological systems. Atomic-resolution simulations are highly complementary to experiments, and can provide data with unparalleled resolution in time and space. Due to the long timescales of biologically relevant events, as well as the complexity of the energy function, accurate and precise simulations remain highly computationally challenging. This seminar will highlight recent progress in both areas, illustrating how energy functions that have been trained on simple peptide models can be successfully used for the study of much more complex systems. We demonstrate that our newly trained energy parameters significantly reduce the secondary structure bias reported for previous Amber parameter sets. Applications of the parameters include studies of folding behavior of peptides and small proteins, and the dynamic behavior of larger biomolecular systems such as conformational changes during drug binding in HIV-1 protease.

1:39PM J6.00005 Beyond force fields. QM/MM conformational searches in biomolecules using Replica Exchange molecular dynamics\(^1\), ADRIAN ROITBERG, Department of Chemistry, University of Florida — Force fields have been extremely successful for our understanding of structure, energetics and dynamics of biomolecules. However, they neglect, for the most part, quantum effects such as charge transfer and polarization. In this talk I will present our work using our newly developed QM/MM interface in the program Amber, which can very efficiently treat small peptides in explicit solvent using a number of different semiempirical methods. We use Replica Exchange molecular dynamics to sample the surface properly and ensure convergence. A comparison of the conformational space sampled by different semiempirical methods in explicit water classical models will be presented. The computational results will be compared against NMR experiments.

Tuesday, March 11, 2008 11:15AM - 2:15PM
Session J7 FEd: Undergraduate Nanotechnology and Materials Physics Education I

Morial Convention Center R05
11:15AM J7.00001 NCLT Contributions to Nanoscience Education at the Undergraduate Level. ROBERT CHANG, Northwestern University — The National Center for Learning and Teaching in Nanoscale Science and Engineering (NCLT) has a mission to build national capacity in Nanoscale Science and Engineering Education (NSEE) by reaching to millions of learners. This mission calls for the development of a globally competitive national nano workforce and national cadre of leaders in NSEE. Part of the NCLT’s integrated program focuses on higher education initiatives and the development of undergraduate resources in NSE. The Center has developed an online educational resource repository for the NSEE community, the NanoEd Resource Portal at http://www.nclt.us. This talk involves a description of the applications and context for integrating NSE into undergraduate courses. It will provide research and development examples on new degree programs and concentrations in NSEE. The following are a few highlights of NCLT’s contributions in undergraduate education:

- Example of several short introductory units on Scanning Tunneling Microscopy, Scanning Electron Microscopy and Nanopatterning Techniques
- Simulations that can be incorporated into undergrad courses on Information Storage Technology (i.e. Nanomagnetism simulations and accompanying introductory material)
- Archive of seminars on various topics on NSE concepts
- Working prototype of Nanoconcentration in Physics
- Database of Degree Programs highlighted on the NCLT NanoEd Resource Portal
- Rubric for course development criteria
- Potential venue for professors to post their courses, degree programs, etc. for national and global dissemination

1NCLT support provided by the National Science Foundation Grant # 0426328.

11:51AM J7.00002 A Cutting-Edge Education: Incorporating Nano into the Undergraduate Curricula. GREG M. ZENNER, University of Wisconsin-Madison — The Interdisciplinary Education Group (IEG) of the Materials Research Science and Engineering Center (MRSEC) on Nanostructured Interfaces at the University of Wisconsin-Madison (UW) develops and uses hands-on, interactive education and outreach materials to engage a variety of audiences in learning about nanotechnology and advanced materials. Many of the education products created are inspired by UW MRSEC research; and faculty, staff, and students regularly contribute to the IEG’s work to share nanotechnology with a broader audience. The UW MRSEC has developed numerous teaching modules, labs, and education resources devoted to nanotechnology concepts, and many of these materials have been integrated into key introductory and advanced undergraduate courses at UW and other institutions, including small liberal arts colleges and community colleges. This effort has taken place through both the creation of new courses and the modification of existing courses to include cutting-edge content based on current research and emerging applications in nanotechnology. In this talk, I will present some of the new instructional materials we have developed based on advances in nanoscale science and technology, the implementation and integration of these materials into undergraduate curricula, and an overview of the UW MRSEC education efforts.

12:27PM J7.00003 Integrating Condensed Matter Physics into a Liberal Arts Physics Curriculum. JEFFREY COLLETT, Department of Physics, Lawrence University, Appleton, WI — The emergence of nanoscale science into the popular consciousness presents an opportunity to attract and retain future condensed matter scientists. We inject nanoscale physics into recruiting activities and into the introductory and the core portions of the curriculum. Laboratory involvement and research opportunity play important roles in maintaining student engagement. We use inexpensive scanning tunneling (STM) and atomic force (AFM) microscopes to introduce students to nanoscale structure early in their college careers. Although the physics of tip-surface interactions is sophisticated, the resulting images can be interpreted intuitively. We use the STM in introductory modern physics to explore quantum tunneling and the properties of electrons at surfaces. An interdisciplinary course in nanoscience and nanotechnology is open to all majors in science and engineering, especially those in second and third year who are interested in future careers in science and technology. This general education course is team-taught with chemists to present recent advances in nanoscale science and technology, the implementation and integration of these materials into undergraduate curricula, and an overview of the UW MRSEC education efforts.

1Work supported by grants from the W.M. Keck Foundation and the NSF-NUE program.

1:03PM J7.00004 Engaging undergraduate students in interdisciplinary courses in nanotechnology. FIONA GOODCHILD, University of California, Santa Barbara — Two new courses at UCSB engage both undergraduate and graduate students in situated learning so that they can acquire the knowledge and skills they will need for future academic courses and career development. These courses are designed and taught by research faculty and education staff at the California Nanosystems Institute (CNSI) at UC Santa Barbara. The speaker, Dr. Goodchild, Education Director at CNSI, collaborated in the course design and is advisor on assessment and pedagogy for both courses. The first course, entitled INSITES, is aimed at first and second year students who are interested in the impacts of science and technology in society. This general education course is team taught by three Graduate Teaching Scholars from across engineering, science and social sciences. They collaborate with lead faculty from Materials Science and History to design both the curriculum and instructional format for the 10 week course that is supported by the National Science Foundation. INSITES was taught for the first time in Spring 2007 and feedback indicated that the course had convinced the undergraduate students that they would like to take further courses outside their majors. The second course, entitled the Practice of Science is open to all majors in science and engineering, especially those in second and third year who are interested in scientific research and related career opportunities. The course has been taught for the past 4 years as a two-quarter course by two research faculty who focus on the nature of scientific discovery, the role of graduate researchers and faculty, the challenges of collaboration across disciplines and the mechanisms for funding research in academia and industry. In the first quarter each students is expected to identify a mentor and a research group in which they can pursue an individual research project, to be completed during the second quarter when the classes are designed to operate like research group meetings. Evaluation indicates that both courses attract students from underrepresented groups in science who value gaining a broader perspective about nanotechnology and the career opportunities that it offers to undergraduate students.
11:15AM J8.00001 Washboard Road: The dynamics of granular ripples formed by rolling wheels. NICOLAS TABERLET, ANNE-FLORENCE BITBOL, ENS Lyon, France, STEPHEN MORRIS, University of Toronto. JIM MCELWAIN, University of Cambridge — We report laboratory experiments on rippled granular surfaces formed under rolling wheels. Ripples appear above a critical speed and drift slowly in the driving direction. Ripples coarsen as they saturate, and exhibit ripple creation and destruction events. All of these effects are captured qualitatively by 2D soft particle simulations in which a disk rolls over smaller disks in a periodic box. The simulations show that compaction and segregation are insensitive to the ripple phenomenon. We describe a simplified scaling model which gives some insight into the mechanism of the instability.

11:27AM J8.00002 Evolution of sand ripples in pulsed flow. JOSÉ EDUARDO WESFREID, CNRS, JOACHIM KRUITHOEF, PMMH - CNRS — We present high-resolution experiments showing the temporal evolution of sand ripples formed by oscillatory flow. We discuss the decompaction process observed during the formation of the ripples pattern. We have also studied the evolution of different parameters during the transition of rolling grain ripples to vortex ripples, as the slope of these ripples and we tested the validity of the Sleath criterion to discriminate the transition.

11:39AM J8.00003 Granular Erosion of Pebbles. ADAM ROTH, DOUGLAS DURIAN, University of Pennsylvania — Flowing grains are strongly abrasive, and cause erosion both of themselves and their surroundings. In a geophysical setting, the erosion of pebbles has traditionally been quantified by global measures such as aspect ratio. Recently we have focused on curvature, and its distribution around the contour, as a local measure more directly related to the microscopic action of erosion. Here we apply this method to linoleum shapes, eroded by rotation in an abrasive grit. Several shape parameters are measured at different stages in the erosion process, including the curvature distribution. A simple model of erosion is developed, and its predictions are compared to the data. The results are in reasonable agreement, and could be useful for understanding natural erosion processes.

11:51AM J8.00004 Impact and Penetration of Granular Materials by Discrete Element Simulations. JUSTIN W. GARVIN, Air Force Research Lab, JEREMY B. LECHMAN, J. MATTHEW D. LANE, Sandia National Labs — Granular materials are an important example of hfi fields, discrete materials deliver 1) to meteorite collision and crater formation. Recently a model for the force experienced on a penetrator has been proposed [L.S. Tsimring and D. Volvon, Powders and Grains 2005, 1215-1223] and shown to fit experimental data well [H. Katsuragi and D.J. Durian, Nature Physics, Vol. 3, June 2007]. This model describes two components of the force: i) a velocity dependent, depth independent term related to the inertial force required to mobilize a volume of grains in front of the penetrator; and ii) a velocity independent, depth dependent, Coulomb friction-like term. In the current study, massively parallel, discrete element simulations have been performed to study the penetration of a large spherical impactor into a multi-million particle bed of granular material. Results agree with previous work for slow impact speeds (< 400cm/s). In addition, the current work extends the comparison with the proposed model to higher speeds (~1000cm/s). The physics of the phenomenon is discussed along with the challenges for modeling and simulation in the even higher velocity regime.

12:03PM J8.00005 Gas-Mediated Impact Dynamics in Fine-Grained Granular Materials. JOHN ROYER, ERIC I. CORWIN, BRYAN CONVYERS, MARK L. RIVERS, PETER J. ENG, HEINRICH M. JAEGGER, James Franck Institute, University of Chicago — Non-cohesive granular media exhibit complex responses to sudden impact that often differ from those of ordinary solids and liquids. We investigate how this response is mediated by the presence of interstitial gas between the grains. Using high-speed x-ray radiography we simultaneously track the motion of a steel sphere through the interior of a bed of fine-grained granular material and measure local changes in the bed packing density below the sphere. In an initially loosely packed granular bed, the sphere causes a near-instantaneous compaction of the bed below itself and an increase in the bulk density of the bed immediately above it. The interstitial gas plays the opposite role, strengthening the bed and inhibiting the penetration of the sphere. These two seemingly incongruous effects are both due to the low permeability of the fine-grained bed, which traps the interstitial gas in the bed. This trapped gas resists changes in the bed packing density, inhibiting compaction in the loose bed and inhibiting dilution in the dense bed.

This work was supported by NSF through DMR-MRSEC and by DoD/AFSOR.

12:15PM J8.00006 Impact cratering in fluidized granular matter. PATRICK MAYOR, HIROAKI KATSURAGI, DOUGLAS J. DURIAN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — Impacts by projectiles dropped into granular media are an important example of how particulate materials respond to externally applied forces. Beyond the obvious geophysical case of planetary craters, understanding the details of impact mechanisms can provide valuable information on these systems, and the phenomenon has been actively investigated. In particular, recent experiments have studied the penetration depth of projectiles impacting granular materials at relatively low speeds, and measured the dynamics of the impact process, yielding force laws accounting for the observations. We have studied how the impact phenomenon is affected when the granular medium is submitted to a vertical upward (or downward) gas flow, in a range of flow rates below the bubbling regime. These fluidized granular systems yield, logically, deeper impacts, and dynamics measurements reveal that the stopping time is also longer, contrary to what is observed when deeper craters are obtained by increasing the impact velocity. We observe that the parameters involved in previously obtained force laws are modified in a simple way as a function of the flow rate and find a velocity-dependent inertial term and a depth-dependent friction force that vanishes as the flow rate approaches the fluidization threshold.

12:27PM J8.00007 Drag Force in a Gas Fluidized Granular Bed. T.A. BRZINSKI, D.J. DURIAN, University of Pennsylvania, Dept. of Physics — We use a rheometer to measure the torque acting on a rotating bar in a bed of gas-fluidized glass beads. We vary rotation rate from .001-100ps, vary depth from 1-10 cm, and increase the fluidizing gas flow from no flow well into the fluidized regime. We observe that at high rotation rates the drag is roughly proportional to velocity squared. At low rates we can resolve the measured torque by depth, and observe a collapse of the data. These results agree with the predictions of a granular drag force model which has proven effective in predicting granular impact dynamics. The model consists of an inertial drag term, which is depth-independent and scales as velocity squared, and a frictional drag term, which is independent of rate and varies linearly with depth. We find, as expected, that while the frictional term is airflow-dependent the inertial term is uncoupled from the fluidization.
12:39PM J8.00008 Exploring penetration through granular media

DANIEL J. COSTANTINO, Department of Physics; Pennsylvania State University, THOMAS J. SCHEIDEMANTEL, MATTHEW B. STONE, JULIA COLE, CASEY CONGER, KIT KLEIN, MATTHEW LOHR, WILLIAM MCCONVILLE, ZACHARY MODIG, KRYSSEN SCHEIDLER, PETER SCHIFFER — The motion of objects through granular media is an important physical problem involving local jamming of the grains. We report on an experiment dealing with the force needed to initiate upward motion through a granular pile, \( F_{\text{in}} \). As expected, this force scales monotonically with the depth of the intruder as well as its size, \( D_{\text{plate}} \). However, unlike previous experiments this force also depends on the size of the particles making up the pile, \( d_{\text{grain}} \). The force can be represented by the function \( F_{\text{in}} = AD_{\text{plate}}^{-2} d_{\text{grain}}^{-2} + BD_{\text{plate}}^{-2} \), which can be qualitatively explained within a simple model. Finally, preliminary results from a new experiment dealing with horizontal motion through a granular pile will be discussed. In this study, the effect of interstitial fluids on a granular material’s resistance to an intruder will be investigated. Research supported by NASA grant NAG-2384 and the NSF REU program.

12:51PM J8.00009 Fluctuations in an agitated granular fluid

KIRI NICHOL, MARTIN VAN HECKE, Leiden University — The clogging of granular materials at the exit of a silo or hopper is a matter of tremendous practical importance, as well as a canonical example of jamming. We investigate the effect of particle aspect ratio (length/width) on the jamming probability through experiments and discrete element simulations. Preliminary experimental results on particles with aspect ratios of 16 and 32 show that the probability of \( P(m) \) for \( m \) grains to exit the hopper has an exponentially decaying tail that, when scaled by the mean number that exit, is independent of exit aperture size. This scaling of \( P(m) / m \) is also observed in hopper flow of ordinary round particles, but the proposed phenomenological explanation of uncorrelated behaviors seems unlikely in long, thin rods. Furthermore, while the mean exit number obviously increases with aperture size, it is not clear which length scale is most relevant: particle length, width, or some combination of the two. We are also writing new discrete element simulations that can be compared with the experiments, and I will discuss some of the computational nuances introduced by particle asymmetry and present initial results.

1:03PM J8.00010 Jamming in Hopper Flow of Large Aspect Ratio Granular Materials

SCOTT FRANKLIN, Rochester Institute of Technology — The clogging of granular materials at the exit of a silo or hopper is a matter of tremendous practical importance, as well as a canonical example of jamming. We investigate the effect of particle aspect ratio (length/width) on the jamming probability through experiments and discrete element simulations. Preliminary experimental results on particles with aspect ratios of 16 and 32 show that the probability of \( P(m) \) for \( m \) grains to exit the hopper has an exponentially decaying tail that, when scaled by the mean number that exit, is independent of exit aperture size. This scaling of \( P(m) / m \) is also observed in hopper flow of ordinary round particles, but the proposed phenomenological explanation of uncorrelated behaviors seems unlikely in long, thin rods. Furthermore, while the mean exit number obviously increases with aperture size, it is not clear which length scale is most relevant: particle length, width, or some combination of the two. We are also writing new discrete element simulations that can be compared with the experiments, and I will discuss some of the computational nuances introduced by particle asymmetry and present initial results.


H. KING, D. ERTAS, A. KUSHNICK, F. ZHOU, ExxonMobil, P. CHAIKIN, NYU — Gravity-driven flows of granular materials are often influenced by interstitial fluids. Using the rotating half-filled drum geometry, we investigated particle and fluid velocities for granular flows of nearly monodisperse spherical glass particles with interstitial fluids of varying dynamic viscosity (air to 4 cP). We utilize direct particle imaging and PIV methods. For dry flows the fundamental time scale is set by the gravitational constant and particle size. We observe two primary influences of the interstitial fluid on the granular rheology. First, density of the fluid changes both the driving force (due to buoyancy) and the inertial response (due to added mass), increasing the characteristic time scale. Second, the intrinsic time scale is influenced by the dynamic viscosity of the fluid. As a result, the changes associated with the 1 cP viscosity increase in going from air-to-water are considerably larger than those for subsequent viscosity increments. We also see that the surface drag associated with the fluid boundary layer progressively affects the grain velocity profile near the surface as the viscosity increases, giving a several-particle-deep zone of constant velocity.

1:27PM J8.00012 Rheology and structure of granular flows in split-bottom geometries

JOSHUA DIJKSMAN, MARTIN VAN HECKE, Leiden University — Combining rheological methods with surface flow imaging, we probe the flow of slow dry granular media as function of driving rate and geometry. The flow rate affects the spatial structure of the flow much stronger than the stresses, while details of the boundary conditions significantly modify both stresses and flow. We discuss our results in the context of recent numerics on rapid flows in these split-bottom geometries, and various theories developed for slow flows.

1:39PM J8.00013 Self-diffusion in bulk sheared granular materials

ANDREEA PANAITESCU, ASHISH ORPE, ARSHAD KUDROLLI, Department of Physics, Clark University — We will discuss the diffusion and structural properties of granular particles in the bulk of a cycledly sheared three dimensional rectangular cell. The particles are visualized away from the side walls using a fluorescent refractive index matched interstitial fluid. Previous studies have shown that the diffusion is anisotropic with respect to the vorticity plane, but these results have been confined to either two dimensional systems or small three dimensional systems where the boundary effects could not be decoupled. In a cyclic shear cell, the packing fraction the particles and their orientational order vary smoothly over time. The particle positions are identified and tracked over long durations to obtain particle diffusivity, mean-squared displacements and probability distributions of particle displacements. An analysis of the effect of structural order on the motion of the particles will be presented.

1:51PM J8.00014 Studies in a 2D granular pure shear experiment

JIE ZHANG, Department of Physics and CNCS, Duke University, NC 27708, USA, PEIDONG YU, TRUSH MAJUMDAR, ROBERT P. BEHRINGER — We have performed two dimensional granular experiments under pure shear using bidisperse photo-elastic disks. Starting from a stress free state, a square box filled with granular particles is subject to shear. The forward shear involved thirty steps, leading to maximum strain of 0.1. The network of force chains gradually built up as the strain increased, leading to increased pressure and shear stress. Backward shear was then applied to return the system to zero strain in the next thirty steps. Following each change of the system, contact forces of individual disks were measured by applying an inverse algorithm. We also kept track of the displacement and angle of rotation of every particle from frame to frame. We present the results for the contact forces, particle displacement, particle rotations, fabric, etc. Work supported by NSF grant DMR0555431.

Tuesday, March 11, 2008 11:15AM - 1:27PM –
Session J9 DFD: Fluid Structure and Properties Morial Convention Center R07

11:15AM J9.00001 The Interplay of Short- and Long-Range Forces in Simulations of Confined Water using Local Molecular Field Theory

JOCELYN RODGERS, JOHN WEEKS, University of Maryland, College Park — A molecular model of water confined between walls is studied using local molecular field (LMF) theory. LMF theory splits the long-ranged Coulomb 1/r potential between charge sites into a short-ranged core potential and a long-ranged, slowly-varying potential ideal for mean-field averaging. The core potential may be treated explicitly by simulations using the minimum image convention with a renormalized external field defined by mean field averaging of the longer-ranged potentials. Here we apply local molecular field theory to molecular dynamics simulations of molecular water confined between walls, with and without an electric field. This is a geometry where short-ranged spherical truncations of Coulomb interactions can fail spectacularly, but in tandem with the effective external field defined by LMF theory such truncations correctly predict structural and electrostatic properties of water. Further the concepts behind LMF theory elucidate the varying contributions of hydrogen-bonding and dipolar interactions in determining the structure of water at surfaces.
11:27AM J9.00002 Effects of a solute on a simple model solvent\(^1\), PAOLO DE GREGORIO, JONATHAN C. TOLEDO, B. WIDOM, Department of Chemistry, Baker Laboratory, Cornell University, Ithaca NY, USA — We studied the effect of the addition of a solute on a one-dimensional model solvent (high density, low compressibility, low coefficient of thermal expansion), at infinite dilution. The solute has a solubility which is low and decreases with increasing temperature. The effect of the addition of solutes on the chemical potential of the solvent at constant volume differs from that at constant pressure in a way similar to that of non-polar solutes in water. The solvent-solute pair distribution function determines fully the modes of decay of the solute-solute counterpart. At the largest distances, the ultimate decay is strictly monotonic (exponential) for both. But while for the solvent-solute correlations the amplitude is strongly associated with the solute solubility, it is negligible for the solute-solute case. Physically, the correlations vanish in identical fashion at infinite distances, but they differ substantially over an extended range of physical interest. The osmotic second virial coefficient is very large and negative, not only as an effect of the proximity ‘attraction’ between the solutes, but also of the very long tail in the correlations.

\(^1\)NSF support is acknowledged.

11:39AM J9.00003 Ultrafast Phase-Contrast Imaging Study of Finite-time Hydrodynamic Singularities\(^1\), YUJIE WANG, Argonne National Lab — Most of the nonlinearity induced hydrodynamic singularities are transient and requires high-speed imaging to be studied. There exist some intrinsic problems of visible-light imaging on fluid mechanical research. The key advantage of x-ray phase-contrast imaging is that it is interface-based technique and the boundaries are highlighted naturally. It is a highly penetrative technique in which all complex structures along the path will be picked up. Additionally, it is naturally immune of the complexity of multiple scattering and strong optical reflection or refraction.

11:51AM J9.00004 Liquid State Properties from \textit{ab initio} Density Functional Theory Calculations\(^1\), NICOLAS BOCK, TRAVIS PEERY, ERIC CHISOLM, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Los Alamos National Laboratory, ERIK HOLMSTRÖM, RAQUEL LIZARRAGA, Instituto de Física, Universidad Austral, Chile — For the solid state, density functional theory (DFT) has been successfully applied to calculate material properties in a large range of materials. In the liquid state however, thermodynamic properties are calculated by molecular dynamics (MD) simulations in which the forces are calculated with DFT. These simulations are computationally significantly more expensive than comparable solid state calculations. We present a novel approach which does not rely on MD simulations, but instead uses Vibration-Transit (V-T) theory to make predictions of the thermodynamic properties of the liquid phase. This approach is computationally significantly less expensive than an MD simulation. The accuracy of this approach is demonstrated by a comparison to experiment.

12:03PM J9.00005 Reconstructing the structure and dynamics of density fluctuations in water near a moving proton, ROBERT CORIDAN, GHEE HWEE LAI, NATHAN SCHMIDT, Department of Physics, University of Illinois, Urbana-Champaign, PETER ABBAMONTE, Department of Physics and Seitz Materials Research Lab, University of Illinois, Urbana-Champaign, GERARD C. L. WONG, Department of Materials Science Engineering, Department of Physics, and Seitz Materials Research Lab, University of Illinois, Urbana-Champaign — The structure and dynamics of water on femtosecond timescales is relevant to many topics in physical chemistry such as ion solvation. We computationally reconstruct the angstrom-scale spatial and femtosecond-scale temporal evolution of density fluctuations in water using high-resolution inelastic x-ray scattering (IXS). The imaginary part of density propagator \(\chi(q,\omega)\) is directly extracted from the IXS data, and the real part recovered using Kramers-Kronig relations. The resultant complex-valued \(\chi(q,\omega)\) is the Fourier transform of the real-space density-density response function \(\chi(r,t)\) which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We use this density propagator from IXS data and linear-response theory to reconstruct the hydration behavior of a proton moving at different instantaneous speeds through water.

12:15PM J9.00006 Classical Density Functional Theory of Inhomogeneous Polar Molecular Liquids, JOHANNES LISCHNER, T.A. ARIAS, Cornell University — We show how free energy functionals for classical assemblies of interacting rigid molecules, composed of an arbitrary number of atoms, can be constructed, such that the entropy of the noninteracting assembly, the thermodynamic properties and the microscopic order of the uniform phase and the dielectric properties in both weak and strong electrostatic fields are reproduced. We use our approach to predict density profiles of liquid hydrogen chlorides in a parallel plate capacitor with different wall potentials and varying external fields. We show that our theory can easily be coupled to electronic structure calculations within the Joint Density Functional approach and will comment on potential application to water.

12:27PM J9.00007 Localized Voronoi analysis of quenched liquid configurations, TRAVIS PEERY, NICOLAS BOCK, GIULIA DE LORENZI-VENNERI, DUANE WALLACE, Theoretical Division, Los Alamos National Laboratory, ERIK HOLMSTROM, Instituto de fisica, Universidad Austral de Chile — We developed a set of localized statistical tools to explore and characterize condensed matter particle configurations, particularly amorphous distributions associated with the liquid state. Typically global measures of atomic packing are used to characterize atomic configurations, such as pair distribution functions. For large systems, such calculations can be computationally expensive and tend not to be sensitive to localized symmetries. Our localized tools are based upon the geometric or topological analysis of (static) atomic arrangements using Voronoi polyhedra. As each atom in the configuration has a unique Voronoi polyhedron defined by its near neighbors, our tools can describe the geometry and symmetry of local neighborhoods. We have defined, for example, a local, Shannon-type entropy for the Voronoi coordination number for each atom in a 500-atom, monatomic system. This localized entropy tool was able to find small (9–40 atom) crystallites or regions of high symmetry in an otherwise random 500-atom configuration quenched from the liquid state. These tools will help to define and characterize not only random liquid state configurations and the minimum structures associated with liquid potential energy surfaces, but also the symmetry properties of the quenching process itself.

12:39PM J9.00008 Phase Separation in the Dipolar Hard-Sphere System Revisited\(^1\), WONKI ROH, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the liquid-vapor transition in the dipolar hard-sphere system. Since the suggestion of de Gennes and Pincus [Phys. kondens. Mater. 11, 189 (1970)] this phase transition has proven both elusive and controversial, with conflicting numerical results regarding its existence and stability. Employing extensive and efficient grand-canonical Monte Carlo simulations, we revisit this issue. High-precision results on the low-temperature heat capacity are presented along isotherms as well as isochores. In addition, we study the density distribution function and its moments for a wide range of chemical potentials, and identify anomalous finite-size effects that can give rise to incorrect conclusions.

\(^1\)This work was supported by the U.S. Department of Energy under Grant No. DE-FG02-07ER46471.

12:51PM J9.00009 X-ray tracer study of Rheology and Hydrodynamics of Fatty acids, MENGNING LIAO, University of Illinois at Urbana Champaign, ROSS HARDER, IAN ROBINSON, University College London, UNICAT TEAM — In wormlike micelles, the breaking and reforming of the micelle rods and the shearing of the rods and between the carbon chains themselves result in a complex diffusive behavior with more than one characteristic time constant. This is one of the characteristics of a Maxwellian fluid. We have studied the rotational Brownian motion of an alumina crystal suspended in a fatty acid liquid. Synchrotron generated hard x-rays are used to do single particle tracking of the rotational orientation by tracking the Bragg intensity of alumina crystals in diffraction geometry. This technique allows the tracking of particles to sub-milladian precision. We have observed multiple time scales of relaxation which is evidence of subdiffusive behavior.
1:03PM J9.00010 Statics and dynamics of a cylindrical droplet under an external body force, JAMES SERVANTIE, MARCUS MÜLLER, Institute For Theoretical Physics, Goettingen — We study the rolling and sliding motion of droplets on a corrugated substrate by Molecular Dynamics simulations. Droplets are driven by an external body force (gravity) and we investigate the velocity profile and dissipation mechanisms in the steady state. The cylindrical geometry allows us to consider a large range of droplet sizes. The velocity of small droplets with a large contact angle is dominated by the friction at the substrate and the velocity of the center of mass scales like the square root of the droplet size. For large droplets or small contact angles, however, viscous dissipation of the flow inside the volume of the droplet dictates the center of mass velocity that scales linearly with the size. We develop a simple analytical description predicting the dependence of the center of mass velocity on droplet size and the slip length at the substrate. In the limit of vanishing droplet velocity we quantitatively compare our simulation results to the predictions and good agreement without adjustable parameters is found.

1:15PM J9.00011 Velocity-dependent friction coefficient at the interface between a polymer melt and a solid substrate, NIKOLAI PRIEZJEV, ANOOSEH NIJAVARNI, Michigan State University — Molecular dynamics simulations are carried out to investigate the dynamic behavior of the slip length in thin polymer films confined between atomically smooth thermal surfaces. For weak wall-fluid interactions, the shear rate dependence of the slip length acquires a distinct local minimum followed by a rapid growth at higher shear rates. With increasing the fluid density, the position of the local minimum is shifted to lower shear rates. We found that the ratio of the shear viscosity to the slip length, which defines the friction coefficient at the liquid/solid interface, undergoes a transition from a nearly constant value to the power law decay as a function of the slip velocity. In a wide range of shear rates and fluid densities, the friction coefficient is determined by the product of the value of surface induced peak in the structure factor and the contact density of the first fluid layer near the solid wall. A relation to recent slip flow experiments is discussed. Reference: A. Njavarni and N.V. Priezjev, Phys. Rev. E (2008) (cond-mat/0711.0187).

Tuesday, March 11, 2008 11:15AM - 2:15PM — Session J10 DCMP: Superconductivity: Vortex I Morial Convention Center R08

11:15AM J10.00001 Progression of the vortex-solid to vortex-liquid phase boundary with oxygen doping in Y_{0.8}Ca_{0.2}Ba_{x}Cu_{y}O_{4} Films, BENJAMIN TAYLOR, RYAN BAUMBACH, M. BRIAN MAPLE, UCSD — By extending magneto-transport measurements to magnetic fields of 35 tesla we have been able to examine the vortex-solid to vortex-liquid transition of thin film Y_{0.8}Ca_{0.2}Ba_{x}Cu_{y}O_{4} samples (6.45 \leq x \leq 7.0) over a field-temperature range larger than heretofore reported. It is found in this work that the shape of the phase boundary, H_{c2}(T), evolves from a very shallow low-field temperature dependence to an extremely rapid high field temperature dependence in the highly underdoped regime (x \approx 6.45). However, in the lightly overdoped regime (x \approx 6.9 - 7.0), H_{c2}(T) displays an increasingly steep low-field temperature dependence followed by a lessening of the steepness of the high-field region as oxygen content increases. This trend suggests that the boundary of the dissipation-less superconducting region of this unconventional high-T_{c} cuprate based compound is evolving in the overdoped state towards a form that is consistent with what is observed in conventional superconductors. This research was supported by U.S. DOE Grant No. DE-FG02-04ER46105. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0084173, by the State of Florida, and by the DOE.

11:27AM J10.00002 Measurements of the anisotropic irreversibility field in the electron-doped high-T_{c} superconductor P_{2-x}Ce_{x}CuO_{4-y}, GUOQING WU, W.G. CLARK, S.E. BROWN, UCLA, R.L. GREENE, U. Maryland, H. BALCI, U. of Illinois, Urbana, A.P. REYES, P. KUHNS, W.G. MOULTON, NHMFL, Tallahassee — We report measurements of the irreversibility field (H_{irr}) in single crystals of the electron-doped high-T_{c} superconductor (HTSC) P_{2-x}Ce_{x}CuO_{4-y} (x = 0.15 and 0.17) with an applied magnetic field (H_{0}) up to 28 T, using the method of the shift in a nuclear magnetic resonance (NMR) probe circuit resonance frequency (f) caused by the susceptibility of the sample. It is observed that for temperatures above 10 K and in the vicinity of H_{0} \perp c, a phase diagram that involves the vortex solid and/or vortex liquid states depending on the alignment of H_{0} relative to the lattice c-axis is proposed, and the obtained anisotropic H_{c2} character along with the evaluated zero T coherence length [\xi_{ab}(0) \parallel c \rightarrow 0] and penetration depth [\lambda_{ab}(0) \rightarrow 0] at H_{0} \parallel c is compared with that of hole-doped HTSCs. This work is supported at UCLA by NSF Grants DMR-0334869 (WGC) and 0520552 (SEB), at U. Maryland by 0352735 (RLG), and NHMFL by 0084173 and the State of Florida.

11:39AM J10.00003 Evolution of Vortex Phase diagram in heavy ion irradiated YBCO, R. XIE, A. RYDH2, U. WELP, W.-K. KWOK, Material Science Division, Argonne National Laboratory, M.R. ESKILDSEN, Department of Physics, University of Notre Dame, LISA PAULIUS, Department of Physics, Western Michigan University — We present a systematic study of the effect of columnar defects induced by heavy ion irradiation on the vortex phase diagram of single-crystal YBCu3O7 using ac-specific heat measurements obtained with a micro-calorimeter. The first order vortex melting line where the vortex lattice transforms into a vortex liquid at intermediate magnetic fields is tracked by the peak in the specific heat. In our pristine untwinned YBCO crystal, the vortex melting line extends from a lower critical point H_{c2}=0.2T to an upper critical point H_{c2}=6T. The crystal was cleaved into several pieces and then irradiated along the c-axis with 1.4GeV Pb ions with different dose matching fields, B_{y}, ranging from 100G to 3000G. We explored the behavior of H_{c1} and H_{c2} in the presence of increasing columnar defects to determine whether the transformation of the first order melting line to higher order occurs abruptly at a defect threshold value or continuously with increasing amount of defects.

1:11PM J10.00004 Evidence for Hexatic Bose Glass in the Mixed Phase of Type-II Superconductors with Material Line Defects, JOSE P. RODRIGUEZ, Physics & Astronomy, California State University at Los Angeles, CHARLES E. CREFFIELD, Fisica de Materiales, Universidad Complutense de Madrid — Dislocation lines and nano-rods inclusions in thin films of YBa_{2}Cu_{3}O_{y} aligned parallel to the c-axis are known to significantly enhance the critical current in external magnetic field that is also aligned in parallel. In contrast to correlated pinning centers created by irradiation, the former material line defects notably arrange themselves in a “liquid” fashion that shows no clusters or voids. Theoretical calculations predict the existence of a hexatic Bose glass at low temperature in such case[1]. We test that prediction by performing Monte-Carlo simulations of the corresponding two-dimensional Coulomb gas ensemble with close to 3000 vortices. In the regime of weak (“liquid”) pinning centers, we find a 2D hexatic vortex liquid at non-zero temperature characterized by isolated edge dislocations. It freezes into a phase-coherent hexatic vortex glass in the zero-temperature limit in accordance with theory [1].


1Research supported in part by the Air Force Office of Scientific Research under grant no. FA9550-06-1-0479.
12:03PM J10.00005 Competition of Point and Correlated Vortex Pinning in Irradiated YBCO\textsuperscript{1}, WAI-KWONG KWOK, ULRICH WELP, JOHN SCHLUETER, RUOBING XIE, Materials Science Division, Argonne National Laboratory, JIONG HUA, ZHILI XIAO, Dept. of Physics, Northern Illinois University, LISA M. PAULIUS, Dept. of Physics, Western Michigan University, MORTEN R. ESKILDSEN, Dept. of Physics, University of Notre Dame. We present a systematic study of vortex pinning on an optimal-doped unwinned YBa\textsubscript{2}Cu\textsubscript{3}O\textsubscript{7-\textdelta} single-crystal irradiated with 1.4 GeV Pb ions and subsequently irradiated with protons. Irradiation to a dose matching field of B\textsubscript{p}=2T completely transforms the first order vortex melting transition to a higher order Bose glass transition. The transformation is also marked by a pronounced increase in vortex pinning at all temperatures, determined from SQUID measurements. We compare the irreversibility line and the remanent moment of the irradiated sample after subsequent irradiation with protons to determine the contribution to vortex pinning from point and correlated defects on the same sample.

\textsuperscript{1}This work was supported by the U.S. Department of Energy, Office of Science, BES - Materials Science and Division of Nuclear Physics (ATLAS) under grant no. W-31-109-ENG-38.

12:15PM J10.00006 Dynamics of driven vortices in type-II superconductors in the presence of strong point or columnar pinning centers\textsuperscript{1}, THANANART KLONGCHEONGSAN, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435, THOMAS J. BULLARD, National Air and Space Intelligence Center, Wright-Patterson AFB, OH 45433-5648, UWE C. TAUBER, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435. We investigate the nonequilibrium steady state of driven magnetic flux lines in type-II superconductors with unidirectional twin boundaries (TBs). We also discuss the matching effect of vortex lattice with TBs, which reflects vortex pinning characteristics of superconductors with TBs. We have studied the dynamics of vortices interacting with unidirectional twin boundaries in a superconductor using molecular dynamics simulation. Current-voltage curves and critical currents have been calculated as a function of vortex density. We found that the critical current as a function of vortex density reveals a staircase pattern and this pattern depends on the pinning strength. This behavior corresponds to discontinuous change of vortex configurations, which reflects vortex pinning characteristics of superconductors with TBs. We also discuss the matching effect of vortex lattice with TBs, and reveal its behavior is different from the one in superconductors with columnar pinning.

\textsuperscript{1}Research in part funded through the National Science Foundation, NSF DMR-0075725.

12:27PM J10.00007 Vortex dynamics and critical current in superconductors with unidirectional twin boundaries, HIDEHIRO ASAI, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo. The pinning of superconducting vortices is important in device applications of superconductors, because immobilization of vortices at pinning sites is essential for lossless transport. Twin boundary (TB) is one of possible candidates for effective pinning centers, in particular in YBa\textsubscript{2}Cu\textsubscript{3}O\textsubscript{7-\textdelta}. Thus, their pinning properties have been actively studied both experimentally and theoretically. However, the pinning characteristics of high-density TBs, which have recently been fabricated successfully, are still unclear. We have studied the dynamics of vortices interacting with unidirectional twin boundaries in a superconductor using molecular dynamics simulation. Current-voltage curves and critical currents have been calculated as a function of vortex density. We found that the critical current as a function of vortex density reveals a staircase pattern and this pattern depends on the pinning strength. This behavior corresponds to discontinuous change of vortex configurations, which reflects vortex pinning characteristics of superconductors with TBs. We also discuss the matching effect of vortex lattice with TBs, and reveal its behavior is different from the one in superconductors with columnar pinning.

12:39PM J10.00008 Non Arrhenius creep motion of interacting vortices in high-\textit{Tc} cuprate superconductors, A. MAEDA, D. NAKAMURA, Dep. Basic Sci., Univ. Tokyo. Dynamics of driven vortices attracted much attention in many different fields of physics. In addition to the understanding of the dynamic phase diagram, the understanding of the elementary process of the vortex motion is crucially important. For a rather large driving force, the existence of a so-called washboard motion has been well established (Y. Togawa et al. : PRL 83 (2000) 3716.). On the other hand, very close to the critical driving force (critical current density), the Anderson-Kim creep picture has been believed for a long time, which is characterized as the Arrhenius process with the linear decrease of the potential barrier as a function of the external driving force. Quite recently, Luo and Hu proposed the possibility of the non-Arrhenius creep process for the vortex motion in Bragg glass phase, based on a numerical simulation (M. B. Luo and X. Hu, PRL98(2007) 267002.). Stimulated by this theoretical work, we performed a detailed \textit{I-V} study in a high-\textit{Tc} cuprate, LSCO, and found (1) The creep process is non-Arrhenius like in the Bragg glass phase. (2) With increasing magnetic field, the creep process changes into the Arrhenius type one suddenly. (3) The field where the process changes roughly agrees with the Bragg-glass-Vortex glass transition, (4) Aging effect of the critical driving force also changes close to the Bragg glass - Vortex liquid boundary. These features agree well with predictions by Lou and Hu.

12:51PM J10.00009 Anisotropy of the Vortex Magnetic Field Distribution in LuNi\textsubscript{2}B\textsubscript{2}, M. R. ESKILDSEN, L. DEBEER-SCHMITT, University of Notre Dame, K. ROVIRA, Florida International University, N. JENKINS, University of Geneva, Switzerland, C. D. DEWHURST, Institut Laue-Langevin, France, S. L. BUD’KO, P. C. CANFIELD, Ames Laboratory and Iowa State University. It is well known that the vortex lattice (VL) symmetry and orientation in type-II superconductors is very sensitive to any anisotropy within the screening current plane. A classic example is the sequence of transitions from hexagonal to rhombic to square symmetry, which was first observed in the borocarbide superconductors and explained by a Fermi surface anisotropy coupled with the non-local electrodynamics responsible for vortex-vortex interactions. Recently, however, this is mounting experimental evidence for a strong gap anisotropy and possible point nodes in the basal plane of these materials. Here we report on small-angle neutron scattering studies of the VL in a carefully annealed, high quality LuNi\textsubscript{2}B\textsubscript{2} single crystal, which permitted us to measure the VL form factor for a large number of reflections. These measurements allow a reconstruction of the real space profile of the magnetic field around the vortices, reflecting the basal plane anisotropy of the screening currents in LuNi\textsubscript{2}B\textsubscript{2}. The results will be compared to predictions for both Fermi surface and gap anisotropies, and will serve as a valuable reference for more complicated compounds as e.g. Sr\textsubscript{2}RuO\textsubscript{4}, heavy fermions and high-\textit{Tc}’s.

1:03PM J10.00010 An infrared study of the pancake vortex state in La\textsubscript{2-\delta}Sr\textsubscript{2}CuO\textsubscript{4} across the phase diagram, ALEXANDER SCHAFGANS, ANDREW LAFORGE, Department of Physics, University of California, San Diego, SASA DORDEVIC, Department of Physics, University of Akron, MUHAMMAD QAZILBASH, Department of Physics, University of California, San Diego, SEIKI KOMIYA, Central Research Institute of Electric Power Industry, Iwato- kita, Komae, Tokyo, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University, DIMITRI BASOV, Department of Physics, University of California, San Diego. We report on a doping dependent study of the far-infrared interlayer response in the high-temperature superconductor La\textsubscript{2-\delta}Sr\textsubscript{2}CuO\textsubscript{4} (La214). A magnetic field up to 8 Tesla applied perpendicular to the CuO\textsubscript{2} planes is found to increasingly suppress the Josephson plasma resonance (JPR) with decreased doping. By 6 Tesla at a temperature of 8 Kelvin, the c-axis reflectivity is identical to that of the normal state in the most underdoped samples, suggesting the sample is in a two dimensional superconducting state. This behavior is in contrast to fields parallel to the CuO\textsubscript{2} planes, where only a small suppression of the JPR is seen up to 17 Tesla. Vortex wandering and static spin density waves are considered as possible mechanisms for plane decoupling.
1:15PM J10.00011 Torque magnetometry on the electron-doped high-temperature superconductor Pr$_{0.88}$LaCe$_{0.12}$CuO$_{4-\delta}$, J.I. OH, P. DHAKAL, Boston College, S. LI, P. DAI, U. Tennessee, M.J. NAUGHTON$^1$, Boston College — We have used cantilever and extraction magnetometry to measure magnetization in optimally doped n-type high-temperature superconductors Pr$_{0.88}$LaCe$_{0.12}$CuO$_{4-\delta}$ ($T_c = 24K$) for magnetic field aligned close to the c-axis, over the temperature range (4K to 300K). We observed a distinct irreversibility line below which the torque magnetization is irreversible. Also, we observed a complex torque behavior where the sign of normal state torque response with field ($dI/dh$) is the same as that of the superconducting counterpart. From dc magnetization experiments, we conclude that superconducting torque signal arises primarily from out-of-plane diamagnetism, whereas in-plane paramagnetism dominates for the normal state.

$^1$Supported by NSF grant DMR-0605339.

1:27PM J10.00012 Vortex pinning and local density of states in an inhomogeneous d-wave superconductor$^1$, DANIEL VALDEZ-BALDERAS, Department of Physics and Astronomy, University of Rochester, DAVID STROUD, Department of Physics, The Ohio State University — We study a model for vortex pinning in a two-dimensional, inhomogeneous, type-II superconductor at low temperatures. The model is based on the Ginzburg-Landau free energy functional with position dependent coefficients, which we chose in such a way that regions with large gap also have large penetration depth. This choice of parameters (suggested by scanning tunneling spectroscopy experiments) results in vortices being pinned by superconducting regions where the gap is large, in contrast to the usual pinning picture. We also compute the density of states of a model BCS Hamiltonian with d-wave symmetry, in which the pairing field is given by the superconducting order parameter appearing in the free energy functional described above. We find that the type of inhomogeneity that we introduce is an indispensable ingredient for our model to reproduce some of the most salient experimental features of the local density of states spectra of cuprates.

$^1$NSF Grant No. DMR04-13395

1:39PM J10.00013 Superconducting Froth$^2$, RUSLAN PROZOROV, ANDREW F. FIDLER, JACOB HOBERG, PAUL C. CANFIELD, Ames Laboratory, Ames, IA 50011 — Studying the structure and dynamics of froths helps to understand the behaviour of complex systems where topological intricacy prohibits exact evaluation of the ground state. Though exact solutions are difficult, general laws that take into account both, the topological constrains and physics and chemistry of the froth matter have been developed. We used low temperature magneto-optical imaging in superconducting lead to add a new member to the froths family, - superconducting quantum froth, in which the boundaries are the superconducting and the interior is the normal phase. Despite very different microscopic origin, the topological analysis of the structure has shown that von Neumann’s and Lewis’ laws apply. Furthermore, for the first time in the froths analysis there is an external global parameter of known behaviour - the total magnetic moment. We show that the statistical laws are in a good agreement with the predicted macroscopic response. We assert that superconducting froth is the new playground for the analysis of complex physics of froths with magnetic field and temperature as tuneable control parameters.

$^2$Supported by the DOE-BES (contract No. DE-AC02-07CH11358) and Alfred P. Sloan Foundation

5:15PM J10.00014 Vortex relaxation of the noncentrosymmetric CePt$_3$Si, A.C. MOTA, Festkoerperphysik, ETH-Zurich, C.F. MICLEA, F. STEGLICH, Max-Planck-Inst. for Chemical Physics of Solids, Dresden, M. SIGRIST, Theoretische Physik, ETH-Zurich, E. BAUER, Inst. für Festkörperphysik, T.U. Wien — The discovery of superconductivity (SC) in CePt$_3$Si by Bauer et al. (PRL 92, 027003 (2004)), has attracted much interest since the compound lacks an inversion center and it has an unusually high upper critical field $H^\text{c}_2$. Theoretical studies have pointed out that spin-orbit coupling could lead to a pairing state of mixed parity. For CePt$_3$Si it has been proposed that the combination of spin triplet p-wave and spin-singlet s-wave symmetries could explain most of the experimental facts consistently. Here we report on flux dynamics on a single crystal of CePt$_3$Si. The SC probed by means of magnetic susceptibility and specific heat shows a sharp transition at $T_c = 0.45 K$ with a width of 0.1 K. Decays of the remnant magnetization display a clean logarithmic time dependence with rates that follow the temperature dependence expected from the Kim – Anderson theory. However, the creep rates are extremely low, lower than observed in any other superconductor. The low rates are not caused by high critical currents. On the contrary, the critical current in CePt$_3$Si is considerably lower than in other superconductors with higher vortex relaxation rates.

2:03PM J10.00015 Model for nodal quasiparticle scattering in a disordered vortex lattice, MARIANNA MALTSEVA, PIERS COLEMAN, Rutgers University — Recent experiments by T. Hanaguri et al. on underdoped Ca$_{2-x}$Na$_x$CuO$_{2}$Cl$_2$ [1] have observed quasiparticle interference effects [2], which are sensitive to the sign of the d-wave order parameter. In a magnetic field, they observe a sizable transfer of scattering weight from quasiparticles to scattering events between anti-nodes of opposite sign to scattering events between anti-nodes of the same sign. We interpret high momentum phase-coherent scattering in terms of the quasiparticle scattering off the vortex walls. The reduction of scattering at even-odd scattering points indicates that the vortices “screen” some of the underlying impurity scattering, as the impurities get trapped inside the vortex cores. [1] T. Hanaguri, Y. Kohsaka, J. C. Davis, C. Lupien, I. Yamada, M. Azuma, M. Takano, K. Ohishi, M. Ono, H. Takagi, cond-mat/0703728. [2] Y. Kohsaka, C. Taylor, K. Fujita, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takano, H. Eisaki, H. Takagi, S. Uchida, J. C. Davis, Science 315, 1380-1385 (2007).


11:15AM J11.00001 Muon spin rotation study of perturbation of the crystalline-electric-field induced by interstitial muon in PrOs$_3$Sb$_{12}$ and PrRu$_3$Sb$_{12}$, LEI SHU, D.E. MACLAUGHLIN, U. of Calif, Riverside, R.H. HEFFNER, Los Alamos National Laboratory, O.O. BERNAL, Calif, State U., Los Angeles, W.P. BEYERMANN, U. of Calif, Riverside, N.A. FREDERICK, W.M. YUHASZ, T.A. SAYLES, T. YANAGISAWA, M.B. MAPLE, U. of Calif, — Muon spin rotation measurements of the temperature dependence of the positive muon Knight shift in single crystals of PrOs$_3$Sb$_{12}$ and PrRu$_3$Sb$_{12}$ reveal a linear scaling of the Knight shift with the bulk magnetic susceptibility at high temperatures. A small deviation from the linear relation appears in PrOs$_3$Sb$_{12}$ below 0.3 K. However, a large magnitude of deviation is observed in PrRu$_3$Sb$_{12}$ below 32 K. The deviation can be explained by the positive muon induced modification of the susceptibility of neighboring Pr$^{3+}$ ions due to a change of the crystalline-electric-field (CEF) splitting. The data indicate that this modification is much smaller in PrOs$_3$Sb$_{12}$ than in PrRu$_3$Sb$_{12}$. A model calculation based on CEF theory is in progress.

$^1$Supported by NSF Grants 0422674(Riverside), 0203524(Los Angeles), 0335173(San Diego), and by DOE DE-FG02-04ER46105 (San Diego)
11:27AM J11.00002 Interplay of superconductivity and rattling phenomena in β-pyrochlore KOs₂O₆ studied by photoemission spectroscopy, TAKAHIRO SHIMOJIMA, YUKI SHIBATA, KYOKO ISHIZAKA, TAKAYUKI KISS, ASHISH CHAINANI, TAKAYOSHI YOKOYA, TADASHI TOGASHI, XIADONG WANG, CHUANGTIAN CHEN, SHUNTORE WATANABE, JUNICHI YAMAURA, SHIGEKI YONEZAWA, YUJI MURAOKA, ZENJI HIROI, TOMOHIKO SAITO, SHIK SHIN, UNIVERSITY OF TOKYO TEAM, THE INSTITUTE OF PHYSICAL AND CHEMICAL RESEARCH TEAM, OKAYAMA UNIVERSITY TEAM, TOKYO UNIVERSITY OF SCIENCE TEAM, CHINESE ACADEMY OF SCIENCE TEAM — The electronic structure near Fermi level of KOs₂O₆ is studied by a laser-excited photoemission spectroscopy. The superconducting(SC) gap clearly opens across the SC transition at 9.6 K, with the strong electron-phonon coupling value of 2Δ(0)/k_BTc ≥ 4.56. Fitting analysis identifies clear anomalies at 7.5 K in the temperature dependences of the SC gap size and the quasiparticle relaxation lifetime. These anomalies and the fine spectral structures arising from phonons, suggest that the existence of the rattling behavior of K ions significantly affects the superconductivity in KOs₂O₆.

11:39AM J11.00003 Controlling physical parameters of layer-structured nitride-halide superconductors, YASUJIRO TAGUCHI, RIKEN — Metal-intercalation into band insulators sometimes affords superconductors, well-known examples of which are carbon-based materials, such as fullerides and graphite. Layer-structured nitride-halide Li₅₋ₓZrNCl and Li₅₋ₓHfNCl (M denotes molecule) belong to another class of intercalation-induced superconductors with relatively high Tc, in which doping level and interlayer distance (and hence interlayer hopping interaction) can independently be controlled by changing Li concentration and the size of the co-intercalated molecule. The controllability provides a unique and interesting opportunity to investigate the effect of the two important physical parameters on Tc in a single system. Recent progress in the synthesis technique enabled us to obtain for the first time a series of single-phase samples of Li₅₋ₓZrNCl with finely controlled doping-levels which were notoriously difficult to prepare. Using these samples, we have established[1] an electronic phase diagram to find anomalous doping evolution of Tc, which takes a maximum value on the verge of superconductor-insulator transition. Based on this phase diagram and the results of systematic Raman scattering and transport measurements, we will discuss possible roles in producing relatively high Tc played by charge fluctuation and reduced disorder scattering in the layered structure reminiscent of modulation-doped semiconductors. We will also briefly refer to our very recent results on the Hf-based materials in which both of the doping level and interlayer distance were varied.


12:15PM J11.00004 Independent control of carrier concentration and interlayer spacing in Li₂HfNCl layered superconductors, TAKUMI TAKANO, ATSUSHI KITORA, TSUKASA KISHIUME, Institute for Materials Research, Tohoku University, YASUJIRO TAGUCHI, FRS-CMGR, RIKEN, YOSHIHITO IWASA, Institute for Materials Research, Tohoku University, INSTITUTE FOR MATERIALS RESEARCH, TOHOKU UNIVERSITY, SENDAI 980-8577, JAPAN TEAM, FRS-CMGR, RIKEN, WAKO, Saitama 351-0198, JAPAN TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY CORPORATION, KAWAGUCHI 352-0012, JAPAN COLLABORATION — Alkali-metal and organic molecule co-intercalated HfNCl is a new class of layered superconductors with relatively high transition temperature (Tc) of 25.5 K. Recently, we have succeeded in synthesis of single phase samples of Li₅₋ₓHfNCl with a wide range of doping concentration of 0.10 ≤ x ≤ 0.50, where we are able to, continuously and independently, control the carrier density and interlayer distance d between the conducting Hf-N layers by means of co-intercalation of Li and organic molecule. Without any molecule, superconductivity appears at x ≈ 0.15 and Tc is almost constant against x above this critical value. Furthermore, we found that Tc is enhanced (~30%) from 20 K to 25.5 K with increasing of d.

12:27PM J11.00005 Unconventional superconductivity in single crystal Lu₂Fe₃Si₂[1], R. GORDON, M.D. VANNETTE, C. MARTIN, Ames Laboratory, T. TAMEGAI, Y. NAKAJIMA, Department of Applied Physics, The University of Tokyo, Japan, R. PROZOROV, Ames Laboratory — Dynamic magnetic susceptibility for a single crystal of the ternary superconductor Lu₂Fe₃Si₂ has been measured using a tunnel diode resonator (TDR) technique. The London penetration depth exhibits non-exponential temperature dependence. We analyze the obtained superfluid density by comparing models of two-gap superconductivity, a gap with nodes or a highly anisotropic gap. The upper critical field is highly anisotropic and is unusually large. Furthermore, hysteresis in the susceptibility implies unusually strong temperature dependence of the critical current. The results are discussed in terms of possible unconventional behavior of this low-Tc superconductor.

1[1]Supported by the DOE-BES (contract No. DE-AC02-07CH11358) and the Alfred P. Sloan Foundation.

12:39PM J11.00006 Two-Gap Superconductivity in Lu₂Fe₃Si₂, TSUYOSHI TAMEGAI, YASUYUKI NAKAJIMA, GUOJIL LI, Department of Applied Physics, The University of Tokyo — Lu₂Fe₃Si₂ is a superconductor with Tc ≈ 6 K containing nonmagnetic iron. Anomalous temperature dependence of specific heat in the superconducting state has been reported in polycrystalline samples; reduced specific heat jump at Tc and apparent residual T-linear term in the limit of T = 0 K. We have successfully grown high-quality single crystals of Lu₂Fe₃Si₂ using the floating-zone technique, and characterized its superconducting and normal state properties. The anomalies of the specific heat reported in polycrystalline samples are reproduced in the single crystals. In addition, we find a second drop of the specific heat below 1 K. We can fit the temperature dependence of the specific heat by assuming two superconducting gaps as in the case of MgB₂. Temperature dependence of Hall coefficient is nonmonotonic, and also suggests the presence of multiple bands in this compound.

12:51PM J11.00007 Point-contact Andreev reflection tunneling spectroscopy (PCARTS) of the superconducting gap structure in LuNi₅B₂C, XIN LU, W.K. PARK, L.H. GREENE, Physics and FSMRL, UIUC, SUNMOK YEO, KYU-HWAN OH, SUNG-IK LEE, Pohang, Korea, SERGEY L. BUD’KO, PAUL C. CANFIELD, Ames Lab and ISU — The PCARTS technique is employed to investigate the gap anisotropy and proposed existence of point-nodes in LuNi₅B₂C (Δc ≈ 18 K). Differential conductance spectra are taken from two different sets of single crystal samples along three major orientations: [001], [110], and [100]. Analyzing using the single-gap Blonder-Tinkham-Klapwijk (BTK) model reproduces shows the gaps along these directions are 2.4, 2.6, and 2.3 meV, respectively, for one set of samples and 2.4, 2.8, and 2.7 meV, respectively, for the other set. This is smaller than the gap anisotropy reported by other groups[1]. At low temperatures, the single-gap BTK model does not satisfactorily fit our data. Models employing an anisotropic gap are being investigated, as are experiments parameterizing the tunneling cone effect.


1Supported by the U.S. DoE DEFG02-91ER45439 through FSMRL and CMM at UIUC and NSF DMR 07-06013 and by DoE DE-AC02-07CH11358 at Ames Lab.
1:03PM J11.00008 Anisotropic properties of aligned weak-ferromagnetic superconductor Ru$_3$Sr$_2$GdCu$_2$O$_8$ — H.C. KU, B.C. CHANG, C.H. HSU, Y.F. CHEN, M.F. TAI, Department of Physics, National Tsing Hua University, Hsinchu 300, Taiwan, Republic of China. SUPERCONDUCTIVITY AND MAGNETISM LABORATORY TEAM — The ab-plane aligned powder in epoxy matrix for the tetragonal Ru$_3$Sr$_2$GdCu$_2$O$_8$ weak-ferromagnetic superconductor was achieved using a field powder alignment method with ab-plane parallel to the applied magnetic field. The c-axis aligned powder can also be obtained using the field-rotation method where c-axis is perpendicular to the applied magnetic field and along the rotation axis. The temperature dependence of magnetic moment m (T) for the aligned powder provides the desired anisotropic properties where larger magnetic moment along the ab-plane was observed. The field-cooled (FC) and zero-field-cooled (ZFC) data in low applied field (1 G) for both directions indicate a weak-ferromagnetic (canted-antiferromagnetic) transition of Ru moment at $T_X$(Ru) = 131 K and a superconducting transition in the Cu$_2$O$_8$ plane at $T_c$ = 39 K. The low temperature antiferromagnetic ordering of the rare earth Gd moment is observed at $T_X$(Gd) = 2.5 K. Diamagnetic superconducting shielding signal is much weaker than bulk sample due to small powder diameter (1-10 $\mu$m), long penetration depth $\lambda$ and the two-dimensional (2D) character of Cu$_2$O$_8$ plane. Low temperature, low field magnetization data m(B, T) will be discussed.

1:15PM J11.00009 Order parameter suppression and structure of the surface states in noncentrosymmetric superconductors — ANTON VORONTSOV, University of Wisconsin-Madison, ILYA VEKHTER, Louisiana State University, MATTHIAS ESCHRIG, Universitaet Karlsruhe. We consider the structure of the surface states at the pairbreaking boundaries of non-centrosymmetric superconductors. In the region of the order parameter suppression multiple Andreev reflections significantly modify the energy and the intragap density of states due to bound states. We elucidate the physics behind this modification by considering a simple model of gap suppression, and comparing it with a fully self-consistent microscopic calculation. We emphasize the experimentally relevant consequences of the lack of inversion symmetry for the surface states. As the discontinuity in the spin-orbit coupling at the boundary makes the interface spin-active, we analyse the resulting spin structure of the bound states.

1:27PM J11.00010 Superconductivity in Sn(1-x-d)In(x)Te and Pb(1-y)Tl(y)Te — ANN ERIKSON, THEODORE GEBALLE, IAN FISHER, Stanford University. Recent evidence for a charge-Kondo effect in superconducting samples of Pb$_{1-y}$Tl$_y$Te [PRL 94, 157002 (2005)] raises the possibility that systems of degenerate semiconductors doped with valence skipping elements may be an ideal realm in which to study suggested negative U pairing mechanisms in superconductors [PRL 61, 2713 (1988)]. However, questions of exactly how the proposed charge-Kondo behavior relates to superconductivity in Pb$_{1-y}$Tl$_y$Te remain. In this work, we study the relationship between the DOS at the Fermi level and Tc in the related superconductor Sn$_{1-x-d}$In$_x$Te, where enhancement of Tc is found above a critical concentration $x_c > d/2$, where the Fermi level is pinned in the impurity band and the DOS is enhanced [Phys. Rev. B 28, 612 (1983)]. We find that the elevated DOS is insufficient to explain the enhanced Tc for these samples, suggesting an additional pairing mechanism is involved, such as the negative U mechanism mentioned above.

1:39PM J11.00011 Novel superconductivity in a new noncentrosymmetric superconductor — LEI FANG, XIYU ZHU, GANG MU, HAI-HU WEN, National Lab for Superconductivity, Institute of Physics, CAS — Low temperature specific, resistivity and magnetization are measured in a newly fabricated superconductor. It is found that this material has no central inversion symmetry. Specific heat measurement show that the major part of the system has a s-wave symmetry and the superconducting gap is thus derived. However, when the superconductivity is suppressed by the magnetic field, a further drop of specific heat coefficient is observed just above Tc. This unexpected behavior remains to a very high magnetic field and without any obvious shift of the transition temperature. It is tempting to argue that this drop of specific heat coefficient may be induced by the spin triplet pairs.

1:51PM J11.00012 Superconductivity in the new Platinum Germanides APt$_4$Ge$_{12}$ (A=Sr,Ba,La,Pr) — HELGE ROSNER, ROMAN GUMENIUK, WALTER SCHNELLE, MICHAEL NICKLAS, ANDREAS LEITHE-JASPER, YURI GRIN, Max-Planck-Institute for Chemical Physics of Solids Dresden, Germany — New germanium-platinum compounds with the filled-skutterudite crystal structure were synthesized. Magnetic susceptibility, specific heat, and electrical resistivity measurements find superconductivity in LaPt$_4$Ge$_{12}$ and PbPt$_4$Ge$_{12}$ below ca. 8 K. The parameters of the normal and superconducting states were established. Strong electron-phonon coupling and a crystal electric field singlet groundstate is found for the Pr compound. Electronic structure calculations show a large density of states at the Fermi level, predominantly due to Ge $4p$ orbitals. Similar behavior, albeit with lower Tc, was observed for SrPt$_4$Ge$_{12}$ and BaPt$_4$Ge$_{12}$.

Tuesday, March 11, 2008 11:15AM - 2:15PM
Session J12 DCMP: Experimental Studies of the Heavy Fermion 115 Compounds Morial Convention Center 203

11:15AM J12.00001 3D Fermi Surface Mapping of Ce$_3$RhIn$_5$ — J.D. DENLINGER, Lawrence Berkeley National Lab, F. WANG, J.W. ALLEN, U. of Michigan, M.B. MAPLE, U.C. San Diego, S. ELGAZZAR, P.M. OPPENEER, Uppsala University — Photon-dependent multi-Brillouin zone angle-resolved photoemission (ARPES) measurements are presented for the antiferromagnet heavy fermion bilayer compound Ce$_3$RhIn$_5$. Highly automated Fermi Surface (FS) mapping for excitation energies of 90-120 eV allow visualization of $k_z$-variations of the electronic structure and permit a $k_z$-tomographic determination of the three-dimensional (3D) FS topology with sufficient detail for quantitative comparison to dHvA orbit areas and LDA-predicted topological shapes. In addition to confirming the quasi-2D circular and square topologies centered on the Brillouin zone corner, highly 3D $k_z$-variations are observed along the (100) directions $\Gamma$-X (Z-R). Results are compared to a similar ARPES determination of the 3D electronic structure and FS of the single layer compound CeCoIn$_5$.

11:27AM J12.00002 Anisotropic quantum criticality in heavy-fermion metal CeCoIn$_5$ — RAMZY DAOU, MAKARY TANATAR, Department of Physique, Universite de Sherbrooke, Quebec, Canada, CEDOMIR PETROVIC, Brookhaven National Laboratory, JOHNPIERRE PAGLIONE, Dept. of Physics, University of Maryland, LOUIS TAILLEFER, Dept. of Physique, Universite de Sherbrooke, Quebec, Canada, Canadian Institute for Advanced Research — We previously reported a violation of the Wiedemann-Franz law in the heavy-fermion metal CeCoIn$_5$ when tuned to its quantum critical point, depending on the direction of electron motion relative to the crystal lattice, which points to an anisotropic destruction of the Fermi surface [1]. Here we present new measurements of electric, thermal and thermo-electric transport coefficients which reveal different anisotropic responses. [1] M.A. Tanatar et al., Science 316, 1320 (2007).

1 Supported by the U.S. DOE (DE-AC02-05CH11231 at the Advanced Light Source, DE-FG02-07ER46379 at UM), by the U.S. NSF (DMR-03-02825 at UM) and by the Swedish Research Council (VR) and the European Commission (JRC-ITU).

now at Ames Lab, Iowa
11:39 AM J12.00003 Nature of the superconducting state of CeCoIn$_5$ as revealed by NMR. GEORGIOS KOUTROULAKIS, VESNA MITROVIC, MARC-ANDRÉ VACHON, Brown University, MLADEN HORVATIC, CLAUDE BERTHIER, GHMFL, GEORG KNEBEL, GERARD LAPERTOT, JACQUES FLOQUET, SPSMS — We report low temperature nuclear magnetic resonance (NMR) measurements of the heavy-fermion superconductor CeCoIn$_5$ in high magnetic fields. The effect of the RF penetration on the NMR spectrum for the different parts of the phase diagram is studied. The implications of this study for the nature of a possible inhomogeneous superconducting state, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, are discussed.

11:51 AM J12.00004 Thermal transport in the vortex state of heavy-fermion superconductor CeCoIn$_5$. M.A. TANATAR, J.P. REID, Département de physique, Université de Sherbrooke, Sherbrooke, Canada, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Physics Department of University of Maryland, Washington, DC, USA, C. PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA, LOUIS TAILLEFER, Département de physique, Université de Sherbrooke, Sherbrooke, Canada — The thermal conductivity of heavy-fermion superconductor CeCoIn$_5$ was measured as a function of temperature and magnetic field throughout the vortex state. An anomalous decrease is found in the field dependence at low fields and low temperature. We discuss the origin of this behavior and its possible relation to the presence of uncondensed electrons, found in a previous doping study of this material [1].


12:03PM J12.00005 NMR investigation of a hole doped CeCoIn$_5$. R. R. URBANO, N. J. CURRO, V. A. SIDOROV, J. D. THOMPSON, Los Alamos National Laboratory, Los Alamos-NM, 87545, U. S. A., L. D. PHAM, University of California, Davis-CA, 95616, U. S. A., Z. FISK, University of California, Irvine-CA, 92697, U. S. A. — We have investigated the local environment of In and Co sites of the heavy fermion compound CeCoIn$_{1-x}$Cd$_x$$_5$ ($x = 0.0, 0.10$ and $0.15$) using Nuclear Magnetic Resonance (NMR) and Nuclear Quadrupole Resonance (NQR) measurements. Recently, it was found that Cd-doping acts as an electronic tuning agent in CeCoIn$_5$ and that superconductivity (SC) and antiferromagnetism (AFM) coexist at ambient-pressure for $0.05 < x < 0.15$. It has also been observed on Cd doped compounds that pressure $P$ recovers the SC, ground-state observed for the undoped compound suggesting it as a reversible tuning parameter. In this work we report data indicating that these phases indeed coexist microscopically. The NMR/NQR spectra of In and Co indicate the presence of electronic inhomogeneity, and the spin-lattice relaxation measurements $T_1^{-1}$ suggest that Cd doping induces changes to the low frequency spin dynamics only below $T \approx 5K$. Furthermore, $T_1^{-1}$ measurements for $x = 0.10$ under pressure show a different spin dynamics response in the paramagnetic state, in contrast with the effect of the chemical pressure. We show that chemical doping and pressure are not equivalent.


12:27PM J12.00007 Evolution of the superconducting properties of CeCoIn$_5$ with Yb substitution. D. HURT, C. CAPAN, Z. FISK, Department of Physics & Astronomy, UC Irvine, Irvine, CA, USA, A. D. BIANCHI, Dpt. de physique, U. de Montréal, Montréal, QC, Canada — We report on the evolution of the physical properties of the Yb substitution series starting from the unconventional superconductor (SC) CeCoIn$_5$ to the isostuctural normal metal YbCoIn$_5$. This study was motivated by the recent results of Cd or Hg substitution at the percentage level on the In site in CeCoIn$_5$, which for low concentrations first was shown to lead to the coexistence of antiferromagnetism with SC and to a complete suppression of SC at higher concentrations. At the same time, the lattice constant of YbCoIn$_5$ indicates that Yb enters this compound in a partially valent configuration suggesting that Yb could also be suitable for doping holes into CeCoIn$_5$. In our substitution series we find that the unit cell volume stays roughly constant up to an Yb concentration of about 40 %, after which the cell volume begins to decrease gradually to the value of YbCoIn$_5$. At the same time we observe a gradual suppression of the transition temperature $T_c$ to zero at an Yb concentration of 60 %. Interestingly, the shape of $H-T$-phase diagram remains the same when the axis is scaled with the respective $T_c$ and upper critical field $H_{c2}$, suggesting that the ratio between Pauli $H_p$ and the orbital critical field $H_{c2}$ remains constant.

12:39PM J12.00008 Quantum oscillations in heavy fermion CeRhIn$_5$. HUIQIU YUAN, TUSON PARK, ERIC BAUER, JOE THOMPSON, JOHN SINGLETON, Los Alamos National Laboratory — Construction of Fermi surface is the key to understand the physical properties of variant materials. In correlated electron systems, the heavy carrier mass strongly attenuates the amplitude of quantum oscillations, and, therefore, the Fermi surface sheets from the heavy electrons are usually not observable at low fields. High magnet fields are an indispensable tool to uncover these important features of electronic structure. Furthermore, strong magnetic field above the Neel critical field may lead to the reconstruction or a volume change of Fermi surface in f-electron antiferromagnets (N. Harrison et al. PRL 99, 056401, 2007). Using the unique facilities in the national high magnetic field lab at LANL, in this presentation we will study the quantum oscillations in the heavy fermion compound CeRhIn$_5$ with a field up to 65T.

12:51PM J12.00009 Pressure effect of single ion Kondo temperature in Ce$_{0.02}$La$_{0.89}$RhIn$_5$. H. LEE, V.A. SIDOROV, Los Alamos National Laboratory, Los Alamos, NM 87544, L.M. FERREIRA, Instituto de Fisica Gleb Wataghin, UNICAMP, 13083-970, Campinas, Brazil, T. PARK, F. RONNING, E.D. BAUER, J.D. THOMPSON, Los Alamos National Laboratory, Los Alamos, NM 87544 — Near a critical pressure $P_c \sim 25$ kbar, CeRhIn$_5$ assumes characteristics of CeCoIn$_5$ at atmospheric pressure: they have comparable $T_c$, similar dHvA frequencies, and display quantum-critical behaviors. Many properties of CeCoIn$_5$ can be interpreted within a two-fluid phenomenology in which there are interpenetrating fluids, a localized $f$-electron Kondo gas (energy scale $T_K$) and an interacting Kondo liquid (energy scale $T^*$). We have measured transport properties of Ce$_{0.02}$La$_{0.89}$RhIn$_5$ under pressures to 50 kbar to determine $T_K(P)$, which at $P=0$ is estimated to be $\sim 0.03K$ from specific heat measurements. $T_K(P)$ increases rapidly, reaching $\sim 1.35K$ at 25 kbar, where it becomes comparable to $T_K(\sim 1.8K)$ of CeCoIn$_5$ at $P=0$. A comparison of $T_K(P)$ with $T^*(P)$, determined from the pressure studies of CeRhIn$_5$, reveals the same correlation between $T_K$ and $T^*$ inferred from a two-fluid analysis of CeCoIn$_5$, further supporting the similarity of these two compounds and the two-fluid phenomenology. [1] S. Nakatsuji et al., Phys. Rev. Lett. 92, 016401 (2004).
1:03PM J12.00010 Uniaxial Pressure and the Superconducting Transition of CeIrIn\(_5\)\(^1\), OWEN DIX, ADRIAN SWARTZ, RENA ZIEVE, UC Davis, TODD SAYLES, BRIAN MAPLE, UCSD — We measure the superconducting transition temperature of CeIrIn\(_5\) with applied uniaxial pressure. Heat capacity shows almost no shift in \(T_c\) as pressure is applied along the \(c\)-axis, contrary to the large decrease expected from earlier thermal expansion measurements. With \(a\)-axis pressure, however, \(T_c\) increases about 20 mK per kbar. These results indicate that another factor besides the \(c/a\) ratio has a strong effect on \(T_c\). Furthermore, applied pressure along either crystal axis strongly reduces the size of the heat capacity transition. We will also discuss the effect of uniaxial pressure on the resistive transition, which at ambient pressure occurs at a temperature well above the heat capacity transition. Finally, we present x-ray diffraction measurements correlating our applied pressures with changes in the crystal lattice constants.

\(^1\)Supported by NSF through DMR-0454869.

1:15PM J12.00011 Evolution of the superconducting state through quantum criticality in CeRh\(_{1-x}\)Co\(_x\)In\(_5\), JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, M.A. TANATAR, J.P. REID, LOUIS TAILLEFER, Département de Physique, Université de Sherbrooke, Canada, M.B. MAPLE, Department of Physics and Institute of Pure and Applied Physical Sciences, University of California, San Diego — The Ce-based 115 materials exhibit a host of novel ground states separated by experimentally tunable quantum instabilities. In the single-crystal alloy series CeRh\(_{1-x}\)Co\(_x\)In\(_5\), long range antiferromagnetic order is gradually suppressed upon chemical substitution of Co for Rh and followed by a robust superconducting state extending to the 2.3 K transition of the infamous heavy-fermion superconductor CeCoIn\(_5\). Here we present a thorough study of heat transport measurements of high-quality single crystals of CeRh\(_{1-x}\)Co\(_x\)In\(_5\) for several different superconducting samples spanning both the coexistent magnetic and non-magnetic regions of the \(x\)-\(T\) phase diagram. By extracting the residual (\(T \rightarrow 0\) limit) electronic thermal conductivity of samples at several \(x\) values, we analyze the nature of the superconducting state on either side of the incipient quantum critical point near \(x \approx 0.65\) and study the influence of coexistent magnetism on the pairing state of these materials.

1:27PM J12.00012 Electronic Duality in the Pressure-tuned Quantum Critical Metal CeRhIn\(_5\), TUSON PARK, M.J. GRAF, LEV BOULAEVSKII, J.L. SARRAO, J.D. THOMPSON, Los Alamos National Laboratory — The heavy fermion compound CeRhIn\(_5\) is a prototypical strongly correlated antiferromagnet where the localized 4f electron of Ce hybridizes weakly with ligand electrons. Applying pressure to this material increases hybridization and induces bulk unconventional superconductivity that arises from pressure-enhanced itinerancy of 4f electrons and that simultaneously coexists with large-moment antiferromagnetic order among localized 4f electrons. This microscopic coexistence of local-moment magnetic order and superconductivity in CeRhIn\(_5\) is distinctly different from conventional models that attribute coexisting spin-density wave magnetism and superconductivity to a Fermi-surface instability. Electronic duality, which is unambiguously revealed in the single 4f electron of cerium in CeRhIn\(_5\), is a new framework emerging from strongly correlated electron matter, ranging from the high-\(T_c\) cuprates and heavy fermion superconductors to plutonium.

1Work at Los Alamos National Laboratory was performed under the auspices of the US Department of Energy, Office of Science, and supported by the Los Alamos Laboratory Directed Research and Development program.

1:39PM J12.00013 ABSTRACT Withdrawn –

2:03PM J12.00015 \(d_{x^2-y^2}\) paring symmetry of heavy fermion CeIrIn\(_5\) remote from antiferromagnetic quantum critical point, YUICHI KASAHARA, T. IWASAWA, Y. SHIMIZU, H. SHISHIDO, T. SHIBAUCHI, Kyoto University, I. VEKHTER, Louisiana State University, Y. MATSUDA, Kyoto University, Institute for Solid State Physics, University of Tokyo — Quasi-two dimensional heavy fermion CeIrIn\(_5\) involves two distinct superconducting domes in the phase diagram, which appear as a function of pressure or Rh substitution of Ir. In the analogy to CeCu\(_2\)Si\(_2\), two distinct superconducting domes with different symmetry has been invoked. We report on the results of low-temperature transport of CeIrIn\(_5\) in the second dome, which locates away from an antiferromagnetic quantum critical point. The thermal conductivity is measured under a magnetic field rotated with respect to the crystal axes, which give direct evidence for superconducting gap structure. Clear fourfold oscillation with minima at [110] and [1-10] directions is observed as rotating magnetic field within the basal \(ab\)-plane, while no oscillation is observed within the \(bc\)-plane. In sharp contrast to previous reports that suggested \(E_g\) symmetry with horizontal line node within the \(ab\)-plane \([1]\), our results are most consistent with \(d_{x^2-y^2}\) symmetry with vertical line nodes along the \(c\)-axis. These results imply that two superconducting domes have the same gap symmetry which appears to be mediated by antiferromagnetic spin fluctuations.


Tuesday, March 11, 2008 11:15AM - 2:03PM –

Session J13 DCOMP GSCCM: Focus Session: Simulations of Matter at Extreme Conditions IV: Crystalline Solids, Liquids, and Methods Morial Convention Center 204
11:15AM J13.00001 Structure and dynamics of supercooled liquid silicon under pressure: A first-principles molecular-dynamics study. , TETSUYA MORISHITA, Research Institute for Computational Sciences, National Institute AIST — Recent investigations have suggested that silicon (Si) may exhibit liquid-liquid transitions under pressure and/or supercooling [2]. Here, we report first-principles molecular-dynamics simulations of supercooled liquid Si focusing on the pressure dependence of structure and dynamics [2]. The pair correlation function of deeply supercooled liquid Si (1100 K) for pressures 0 - 18 GPa shows considerable structural changes resulting from the collapse of tetrahedral configurations. The power spectrum of the velocity auto-correlation function also confirms the reduction of the tetrahedral order by pressurization. The self-diffusion coefficient as a function of pressure shows a broad maximum around 10 GPa. However, at a higher temperature (1500 K), the diffusion coefficient simply decreases with increasing pressure, indicating conspicuous dependence of the dynamics and relevant structure upon temperature. [1] T. Morishita, Phys. Rev. Lett. 93, 055503 (2004); ibid. 97, 165502 (2006). [2] T. Morishita, Phys. Rev. E 72, 021201 (2005).

11:27AM J13.00002 Molecular dynamics simulation of the shock-induced wurtzite-to-rocksalt transition in CdSe and CdS1. , AIDAN THOMPSON, MARCUS KNUDSON, Sandia National Laboratories — The shock-induced wurtzite-to-rocksalt structural transformation is studied using large-scale molecular dynamics simulation. The primary goal is to understand the atomicistic mechanisms underlying the interesting transformation kinetics observed in the case of cadmium sulfide [M. D. Kudson and Y. M. Gupta, J. Appl. Phys. v. 91, p. 9561, 2002]. Since the mechanical and structural properties of CdS are very similar to those of CdSe, we have performed multi-million atom MD simulations of the shock-induced phase transformation in CdSe single-crystals using the well-established interatomic potential of Rabani, which has been shown to correctly describe the wurtzite and rocksalt phases and the transformation pressure. In MD simulations of shock along the wurtzite c-axis, the elastically-compressed wurtzite transforms directly to grains of rocksalt. Along the a-axis, a three-wave structure is observed; the wurtzite first transforms to a tetragonal crystal phase, which in turn transforms to rocksalt grains.

11:39AM J13.00003 Large-scale molecular dynamics modeling of shock wave propagation in silicon. , XIANG GU, MIKALAI BUDZEVICH, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology. CARTER WHITE, Naval Research Laboratory — We performed molecular dynamics simulations of shock wave propagation in silicon. The different regimes of materials response were studied as a function of shock wave intensity and crystalline orientation of shock wave propagation. The shock Hugoniot is predicted in a wide range of piston velocities (0-12 km/s), and for several crystallographic orientations <100>, <110>, and <111>. Shock Hugoniots were used for a detailed analysis of a material's response to complex, split shock-wave structures. The special regime of an anomalous response of the material which is characterized by absence of plastic deformation in the intermediate interval of shock wave intensities was investigated.

11:51AM J13.00004 Shock front broadening in polycrystalline materials. , JOHN BARBER, KAI KADAU, Los Alamos National Laboratory — We analyze a model for the evolution of weak shock fronts (or elastic precursor waves) in polycrystalline materials. This model is based on the ideas of Wayers and Carvalho [Mater. Sci. Eng., 292-293 (1976)] that the shock velocity anisotropy within the polycrystal is the most important factor in shock front broadening. Our analysis predicts that the shock front width increases as the 1/2 power of the front penetration distance into the crystal. Our theoretical prediction is in plausible agreement with previous experimental results for the elastic precursor rise time, and it should therefore provide a useful shock width estimate. Furthermore, our theoretical framework is also applicable to other problems involving front propagation in heterogeneous media.

12:03PM J13.00005 Large Scale Molecular Dynamics Simulations of Dense Plasmas. , JEROME DALIGAULT, GUY DIMONTE, Los Alamos National Laboratory. Plasmas are generally created and probed by depositing energy into matter, driving it far from equilibrium. Knowledge over a wide range of physical conditions of the rate at which the electronic and ionic subsystems come into thermal equilibrium is important for explicit practical purposes. The microscopic mechanisms vary with the strength of the coupling among particles and the degree of degeneracy of the electrons. Though a variety of models for the electron-ion energy equilibration rate were proposed, these models apply to specific regimes, their range of validity and the transition from one regime to another remains unclear. Molecular dynamics (MD) simulations provide a powerful tool to investigate the validity of the various models. In order to study the temperature relaxation rates over a wide range of plasma coupling, from very weakly coupled to strongly coupled multi-million particles simulations are necessary. To this end, we have developed a parallel MD code that employs the particle-particle particle-mesh algorithm and allow the simulation of very large, complex Coulomb systems and over long time scales. We have performed detailed, multi-million particle MD simulations to investigate and shed some new light on the electron-ion energy relaxation in hot, dense plasmas. In this talk, we will describe the MD code and discuss the original results obtained for the temperature relaxation rates.

12:15PM J13.00006 Effect of Crystalline Anisotropy on Shock Propagation in Sapphire. , W.J. NELLISS, Harvard U., G.I. KANEL, S.V. RAZORENOV, A.S. SAVINYKH, Russian Academy of Sciences, A.M. RAJENDRAN, U.S. Army Research Office — The major impediment to measuring resoshock temperatures is opacity induced in anvil/windows by shock. We report measured shock profiles of c-, d-, and r-cut single crystals and comparison of these mechanical responses with optical snapshots measured by Hare et al. Profiles were measured at three peak stresses and two sample thicknesses. Particle velocity histories were recorded for sapphire/LIF interfaces. VISAR waveforms are noisy as a result of heterogeneous inelastic deformation and noise depends on crystal orientation and stress amplitude. Heterogeneity is least for r-cut and most for c-cut, which correlates with observed optical heterogeneity. At 2.4 mm thickness r-cut has a three-wave structure that might indicate several elastic-wave speeds off an axis of symmetry. The small signal of the third wave might also indicate a phase transition in the small volume of the sample at higher temperatures. The Hugoniot elastic limit of c-sapphire is defined by the lack of scattered from shot to shot; scatter in the HEL of r- and d-cut are smaller. Radial pre-stressing of c-sapphire resulted in some increase of the rise time of the second wave; no significant effect of pre-stressing was observed for d- and r- samples.

12:27PM J13.00007 Shock Pulse Effects in PTFE Shocked to the Crystalline Phase II–III Transition. , ERIC N. BROWN, Los Alamos National Laboratory, ADWP, GEORGE T. GRAY III, PHILIP J. RAE, Los Alamos National Laboratory, MST-8, NEIL K. BOURNE, AWE, UK — We present an experimental study of crystalline structure evolution of polytetrafluoroethylene (PTFE) due to pressure-induced phase transitions in a semi-crystalline polymer using soft-recovery, shock-loading techniques coupled with mechanical and chemical post-shock analysis. Gas-launched, plate impact experiments have been performed on pedigreed PTFE 7C, mounted in momentum-trapped, shock assemblies, with impact pressures above and below the phase II to phase III crystalline transition. Below the phase transition only subtle changes were observed in the crystallinity, microstructure, and mechanical response of PTFE. Shock loading of PTFE 7C above the phase II–III transition was seen to cause both an increase in crystallinity from 38% to ~53% (by Differential Scanning Calorimetry, DSC) and a finer crystalline microstructure, and changed the yield and flow stress behavior. We particularly focus on the effect of pulse duration on the microstructure evolution.

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DEAC04-94AL85000.

2Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DEAC04-94AL85000.
12:39PM J13.00008 Electrical Breakdown and Lock-On in Photoconductive Semiconductor Switch (PCSS) Devices 1, HAROLD HJALMARSON, KENNETH KAMBOUR, FRED ZUTAVERN, Sandia National Laboratories, CHARLEY MYLES, Texas Tech University — Optically-triggered, high-power photoconductive semiconductor switches (PCSS’s) using semi-insulating GaAs are being developed at Sandia Labs. These switches carry current in high carrier-density filaments. The properties of these filaments can be explained by redistribution of carrier energy caused by carrier-carrier scattering within the filament. This process enhances the impact ionization rate thus allowing these filaments to be sustained by relatively low fields, a process called lock-on. For GaAs, the sustaining field is approximately 4.5 kV/cm. For this talk, the physics mechanisms for lock-on and high-field electrical breakdown are described. Also, a continuum implementation of these physics mechanisms is used to compute the properties of these filaments. These continuum calculations are based on previous calculations in which the filament properties are computed using a Monte Carlo method to solve the steady-state Boltzmann equation.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin company, for the United States Department of Energy under contract DE-AC04-94AL85000.

12:51PM J13.00009 Ideal Strength of Hexagonal Diamond and Related B-C-N Compounds 1, CHANGFENG CHEN, YI ZHANG, University of Nevada, Las Vegas, ZICHENG PAN, HONG SUN, Shanghai Jiao Tong University, China — We have performed first principles calculations on the ideal strength of h-diamond, w-BN, and Φ-BCN. We have considered structural deformation under pure tensile, pure shear or biaxial stress fields. The calculated results reveal new atomistic fracture mechanism for these materials.

1 This work was supported by the Department of Energy Cooperative Agreement DE-FC52-06NA26747 at UNLV and the NNSF of China grants 10574089 and 5053020, Chinese National Minister of Education Program for Innovative Research Team in University at SJTU.

1:03PM J13.00010 Equation of state of crystalline FeO from diffusion Monte Carlo simulations 1, JINDRICH KOLORENC, LUBOS MITAS, North Carolina State University, Raleigh — We investigate equation of state of stoichiometric FeO (at T = 0 K) by means of the diffusion quantum Monte Carlo method (DMC). We find a pressure induced transition from the B1 (rocksalt) structure, which represents the ambient pressure ground state, to the inverse B8 (NiAs) lattice. Experimental evidence for such a transition is still rather controversial, being detected in some measurements and not seen in others. Our DMC estimate for transition pressure, P = 65 ± 5 GPa, is compared to outcome of other computational approaches, such as the density functional theory combined with hybrid exchange-correlation functionals.

1:15PM J13.00011 An efficient method for calculating high PT elastic constants 1, ZHONGQING WU, University of Minnesota — First-principles quasi-harmonic calculations play a very important role in mineral physics because they can accurately predict the structure and thermodynamic properties of materials at pressure and temperature conditions that are still challenging for experiments. It also enables calculations of thermoelastic properties by obtaining the second-order derivatives of the free energies with respect to strain. However, these are exceedingly demanding computations requiring thousands of large jobs running on 10^4 processors each. Here we introduce a simpler approach that requires only calculations of static elastic constants and phonon density of states for unstrained configurations. This approach decreases the computational time by more than one order of magnitude. We show results on MgO and forsterite that are in very good agreement with previous first-principles results and experimental data.

1:27PM J13.00012 Radiation in Particle Simulations of Hot Dense Matter 1, FRANK GRAZIANI, RICHARD MORE, Lawrence Livermore National Laboratory — The variety of complex processes that take place in hot dense radiative plasmas where temperatures are in excess of several keV and densities are higher than metals, has forced computational physicists in ICF and astrophysics to make a number of assumptions regarding how to model non-equilibrium plasmas undergoing thermal relaxation. In order to make the simulations feasible, variations on the Landau-Spitzer model are frequently invoked. There has been recent work on the theoretical properties of thermal relaxation in such plasmas, but there is controversy due to the various approximations needed to make the calculations tractable. Experimental validations in the regimes of interest are prohibitive. Direct Numerical Simulation (DNS) of the many-body interactions of plasmas is a promising approach to model validation but unfortunately, previous work either relies on the collisionless approximation or radiation is entirely absent. We present a new numerical simulation capability that will address a currently unsolved problem: the extension of molecular dynamics to collisional plasmas where Bremsstrahlung and Compton scattering are present. This new tool provides a method for assessing the accuracy of energy and momentum exchange models in hot dense plasmas.

1:39PM J13.00013 Trajectories and escape rates from a collapsing basin: dependence on the rate of collapse of the basin 1, ANTONIO CADILHAC, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; GCEP-Centro de Física da Universidade do Minho, 4710 Braga, Portugal, A.F. VOTER, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545 — It has been shown that trajectories with different initial conditions synchronize in harmonic basins during Langevin-thermostatted molecular dynamics under the same time-noise sequence. Synchronization leads to exponential trajectory coalescence onto a single master trajectory [1]. We present our preliminary results extending previous research to include time dependent harmonic potentials, of the form V(x,t) = A(1 - e^{-αt})V∞, where A, α, and V∞ are constants, which are relevant for understanding the dynamics of driven systems. We present analytical results for the synchronization behavior in the various regimes arising in this context. We also complement the study with numerical estimates of the escape rates for basins with escape paths and compare them to static, conventional rates of escape. [1] Blas P. Uberuaga, Mariang Anghel, and Arthur F. Voter, J. Chem. Phys. 14, 6363 (2004).

1:51PM J13.00014 Momentum Transfer in Soft X-ray - Induced Shock Loading of Meteorite and Planetary Materials 1, JOHN REMO, Harvard University Center for Astrophysics, MICHAEL FURNISH, Sandia National Laboratories — The response of meteorite and planetary materials to high- intensity <1 keV x-rays from Z-pinch sources is described. These materials include iron and stony meteorites, magnesium rich olivine (dunite), and Al and Fe calibration samples. Input stresses varied from 6.1 to 12.4 GPa, attenuating to ~1.4 to 2.5 GPa for the iron meteorites, ~0.3 to 1.9 GPa for the stony meteorites, and 1.64 to 1.91 GPa for dunite. The calibration (pure) metals showed less attenuation than the highly inhomogeneous natural materials. 9.5 to ~5 GPa for Fe and 12.4 to 10.6 GPa for Al. Methods for deducing momentum and energy coupling into these materials from the radiation are discussed. These data are useful for planetary and astrophysical modeling and for near-Earth object mitigation studies requiring momentum coupling, and momentum enhancement coefficients.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Tuesday, March 11, 2008 11:15AM - 2:15PM –
Session J14 DAMOP: Focus Session: Berezinskii-Kosterlitz-Thouless Regime and Rotating Quantum Gases Morial Convention Center 205
11:15AM J14.00001 Kosterlitz-Thouless Transition in Finite-Size BEC Systems¹, GARY WILLIAMS, UCLA — The Kosterlitz-Thouless transition in two-dimensional BEC condensates is calculated taking into account the fact that these are finite-size systems. The outer boundaries of the condensate effectively act as hard walls, and this has a polarizing effect on the vortex pairs. As a consequence the superfluid fraction becomes strongly anisotropic, with the tensor component perpendicular to a wall falling to zero there, while the parallel component remains finite. The decreased pair energy near the walls results in an enhanced vortex density near the boundaries. Possible experiments are proposed to probe the anisotropic properties of the superfluid density, including an unusual sharp dip in the superfluid density that is predicted to occur down the middle of a long superfluid strip.

¹Work supported by the NSF, DMR 05-48521

11:27AM J14.00002 Interference of a stack of coupled two-dimensional BEC pancakes, DAVID PEKKER, VLADIMIR GRITSEV, EUGENE DEMLER, Harvard University — We study the superfluid-normal transition in a stack of Josephson coupled two-dimensional BEC pancakes. Using a combination of the Renormalization Group and the self-consistent harmonic approximation we look at the transition from Kosterlitz-Thouless type behavior to 3D XY type behavior in this finite sized system. We compute the form of the interference patterns that can be observed experimentally if the gas is allowed to expand. In particular, we concentrate on the amplitude modulations in the direction normal to the two-dimensional pancakes, i.e. the direction of fastest expansion.

11:39AM J14.00003 Evolution from BCS to BKT superfluidity in one-dimensional optical lattices, MENDERES ISKIN, CARLOS A.R. SA DE MELO¹, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, Maryland 20899-8423, USA. — We analyze the finite temperature phase diagram of Fermi-Fermi mixtures in one-dimensional optical lattices as a function of fermion-fermion interaction strength. At low temperatures, the Fermi-Fermi mixture evolves from a three-dimensional (3D) Bardeen-Cooper-Schrieffer (BCS) to a two-dimensional (2D) Berezinskii-Kosterlitz-Thouless (BKT) superfluid as the interaction strength increases. We show that the Ginzburg- Landau-Wilson action near the critical temperature is of the Lawrence-Doniach type for all interaction strengths, and explore the phase space of interaction strength versus hopping (or lattice depth) to determine the characteristic line where the behavior of mixture changes from 3D to 2D. Furthermore, we discuss the existence of vortex loop excitations, and how they evolve as a function of interaction strength.

¹School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0432, USA.

11:51AM J14.00004 Berezinskii-Kosterlitz-Thouless Crossover in a Trapped Atomic Gas, ZORAN HADZIBABIC, University of Cambridge — Physics of a Bose gas in 2D is quite different from the usual 3D situation. In a homogeneous 2D fluid of identical bosons long-range order is always destroyed by long wavelength thermal fluctuations and this system cannot undergo conventional Bose-Einstein condensation. Nevertheless, it can become superfluid at a finite critical temperature. This phase transition does not involve any symmetry breaking and in the Berezinskii-Kosterlitz-Thouless (BKT) paradigm it is explained in terms of binding and unbinding of pairs of vortices with opposite circulations. Above the critical temperature, proliferation of unbound vortices is expected. Using optical lattice potentials we can create two parallel, independent 2D atomic clouds with similar temperatures and chemical potentials. When the clouds are suddenly released from the trapping potential and allowed to freely expand, they overlap and interfere. This realizes a matter wave heterodyning experiment which gives direct access to several features of the phase distributions in the two planes. Long wavelength phase fluctuations create a smooth and random variation of the interference fringes and free vortices appear as sharp dislocations in the interference pattern. Both the temperature study of these effects and the measurements of the critical point support the BKT picture of the development of quasi-long-range coherence in these systems.


12:27PM J14.00005 Density Matrix Renormalization Group study of rapidly-rotating two-dimensional bosons¹, DMITRY KOVRIZHIN, Theoretical Physics, Oxford University, 1 Keble road, Oxford, OX1 3NP, United Kingdom — We study a system of two-dimensional bosons with contact interactions in a rapidly-rotating anisotropic trap. The ground state phase diagram and the excitation spectra are investigated using the Density Matrix Renormalization group (DMRG) and the exact diagonalization methods.

¹This work was supported by EPSRC grant EP/D066379/1

12:39PM J14.00006 A vortex dipole in a trapped 2D Bose condensate, WEIBIN LI, MASUD HAQUE, STAVROS KOMINEAS, MPI-PKS Dresden, Germany — We study the dynamics and the stationary states of a vortex-antivortex pair in a two-dimensional Bose condensate in a circular trap. The dynamics of this system turns out to be surprisingly complicated, reflecting the nonlinearity of the underlying Gross-Pitaevskii equation. We use a combination of methods — a time-dependent variational calculation, explicit numerical solutions of the time-dependent and time-independent Gross-Pitaevskii equations, and an exact solution of the non-interacting case — to uncover the physics of the vortex dipole system.

12:51PM J14.00007 Vortex lattices of bosons in deep rotating lattices¹, DANIEL GOLDBAUM, ERICH MUELLER, Cornell University — We study vortex-lattice phases for a Bose gas trapped in a rotating optical lattice near the Mott-Hubbard transition. Unlike the case of shallow lattices, the physics in this regime is dominated by the strong on-site interaction between bosons. We find a series of first-order structural transitions between square lattices where vortices are pinned with their cores on plaquettes/sites. We discuss connections between these vortex structures and the Hofstadter butterfly spectrum of free particles on a rotating lattice. We also investigate vortex configurations in a harmonic trap, where superfluid and Mott phases can coexist in a shell structure.

¹This material is based upon work supported by the National Science Foundation under grant PHY-0450261.

1:03PM J14.00008 Trapped Fermi Gases in Rotating Optical Lattices: Realization and Detection of the Topological Hofstadter Insulator, MEHMET OKTEL, Department of Physics, Bilkent University, 06800, Ankara Turkey, HUI Zhai, Department Of Physics, University of California, Berkeley, California, 94720, USA, ONUR UMCALILAR, Department of Physics, Bilkent University, 06800, Ankara, Turkey — We consider a gas of non-interacting spinless fermions in a rotating optical lattice and calculate the density profile of the gas in an external confinement potential. The density profile exhibits distinct plateaus, which correspond to gaps in the single particle spectrum known as the Hofstadter butterfly. The plateaus result from insulating behavior whenever the Fermi energy lies within a gap. We discuss the necessary conditions to realize the Hofstadter insulator in a cold atom setup and show how the quantized Hall conductance can be measured from density profiles using the Streda formula.
remarking on ways to minimize domain nucleation, identifying algorithms with continuous symmetries and/or nearly fully-connected topologies as promising.

domains. The runtime then grows faster than any polynomial, though it often remains subexponential. We show this via a scaling argument based on the

have finite range interactions in 3 or fewer dimensions, then it is much more likely that they undergo this phase transition in piecemeal fashion by nucleating

quantum phase transition in a homogeneous system, then the runtime is only polynomial in the number of qubits. However, we next show that if the qubits

ically a quantum phase transition point for the computer’s qubits. We show that if the qubits undergo this phase transition simultaneously as in a continuous

Computation

HOWARD BARNUM, LANL — We develop a quantum algorithm to solve combinatorial optimization problems through quantum simulation of a classical

like a huge classical ball that rolls from site to site (for strong attractive interaction). We demonstrate the feasibility of this concept and point out that such

interactions, ranging from a one-by-one transport of atoms (for strong repulsive interaction) to a regime where the particles are are glued together and behave

between adjunct sites of an optical trap. We show that the nature of the transport process depends crucially on the sign and on the strength of the interatomic

into a closed circuit. It produces a DC circulating atomic current in response to a cyclic adiabatic change of the on-site potentials and the tunneling rates

of Physics, Ben-Gurion University, Beer-Sheva, Israel — We propose a BEC stirring device which can be regarded as the incorporation of a quantum pump

Department of Physics, Wesleyan University, CT, USA and MPI for Dynamics and Self-Organization, Goettingen, Germany, DORON COHEN, Department

Department of Physics, Colorado School of Mines, DIMITRI R. DONUNAS-FRAZER, Department of Physics, University of California, Berkeley — We present the complex

quantum dynamics of vortices in Bose-Einstein condensates in a double well via exact diagonalization of a discretized Hamiltonian. When the barrier is high,
vortices evolve into macroscopic superposition (NOON) states of a vortex in either well — a Schrödinger cat with spots. Such Schrödinger leopard states are

more robust than previously proposed NOON states, which only use two single particle modes of the double well potential.

3Supported by the National Science Foundation

1:39PM J14.00011 Vortex lattice transitions in cyclic spinor condensates , SUBROTO MUKERJEE, UC Berkeley, RYAN BARNETT, UC Berkeley — We study the energetics of vortices and vortex lattices produced by rotation in the cyclic phase of $F = 2$ spinor Bose condensates. In addition to the familiar triangular lattice predicted by Tkachenko for $^3$He, many more complex lattices appear in this system as a result of the spin degree of freedom. In particular, we predict a magnetic-field-driven transition from a triangular lattice to a honeycomb lattice. Other transitions and lattice geometries are driven at constant field by changes in the temperature-dependent ratio of charge and spin stiffnesses, including a transition through an aperiodic vortex structure.

1:51PM J14.00012 Condition for the existence of complex modes in a trapped Bose-Einstein condensate with a highly quantized vortex , MAKOTO MINE, ERIKO FUKUYAMA, Department of Physics, Waseda University, MASAHIKO OKUMURA, Japan Atomic Energy Agency, and CREST (JST), TOMOKA SUNAGA, Department of Physics, Waseda University, YOSHIYA YAMANAKA, Department of Electronic and Photonic Systems, Waseda University — We consider a trapped Bose-Einstein condensate (BEC) with a highly quantized vortex. For the BEC, with a doubly, triply, or quadruply quantized vortex, the numerical calculations have shown that the Bogoliubov-de Gennes equations, which describe the fluctuation of the condensate, have complex eigenvalues. In this talk, we show the analytic expression of the condition for the existence of complex modes, using the method developed by Rossignoli and Kowalski$^1$ for the small coupling constant. To derive it, we make the two-mode approximation. With the derived analytic formula, we can identify the quantum numbers of the complex modes for each winding number of the vortex$^2$. Our result is consistent with those obtained by the numerical calculation in the case that the winding number is two, three, or four. We prove that the complex modes always exist when the condensate has a highly quantized vortex$^2$.


2:03PM J14.00013 Control of atomic currents using a quantum stirring device , MORITZ HILLER, MPI for Dynamics and Self-Organization, Goettingen, Germany and Department of Physics, University of Goettingen, Germany, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, CT, USA and MPI for Dynamics and Self-Organization, Goettingen, Germany, DORON COHEN, Department of Physics, Ben-Gurion University, Beer-Sheva, Israel — We propose a BEC stirring device which can be regarded as the incorporation of a quantum pump into a closed circuit. It produces a DC circulating atomic current in response to a cyclic adiabatic change of the on-site potentials and the tunneling rates between adjacent sites of an optical trap. We show that the nature of the transport process depends crucially on the sign and on the strength of the interatomic interactions, ranging from a one-by-one transport of atoms (for strong repulsive interaction) to a regime where the particles are glued together and behave like a huge classical ball that rolls from site to site (for strong attractive interaction). We demonstrate the feasibility of this concept and point out that such device can be utilized in order to probe the interatomic interactions.


11:15AM J15.00001 Quantum simulated annealing , SERGIO BOIXO, UNM, ROLANDO SOMMA, Perimeter Institute, HOWARD BARNUM, LANL — We develop a quantum algorithm to solve combinatorial optimization problems through quantum simulation of a classical annealing process. Our algorithm combines techniques from quantum walks and quantum phase estimation, and can be viewed as the quantum analogue of the discrete-time Markov Chain Monte Carlo implementation of classical simulated annealing.

11:27AM J15.00002 Domain Nucleation as a Failure Mode of Adiabatic Quantum Computation$^1$, WILLIAM KAMINSKY, SETH LLOYD, MIT — The bottleneck limiting the runtime of an adiabatic quantum algorithm is generally a quantum phase transition point for the computer’s qubits. We show that if the qubits undergo this phase transition simultaneously as in a continuous quantum phase transition in a homogeneous system, then the runtime is only polynomial in the number of qubits. However, we next show that if the qubits have finite range interactions in 3 or fewer dimensions, then it is much more likely that they undergo this phase transition in piecemeal fashion by nucleating domains. The runtime then grows faster than any polynomial, though it often remains subexponential. We show this via a scaling argument based on the Suzuki-Trotter mapping. Our argument extends previous similar ones in that it explicitly shows how domain excitations typically must lead to computational errors as inter-domain couplings typically are insufficient to allow the excitations to reconcile with one another and lead back to a valid solution. We close by remarking on ways to minimize domain nucleation, identifying algorithms with continuous symmetries and/or nearly fully-connected topologies as promising.

$^1$This work was supported in part by the Laboratory for Physical Sciences and DoD under the AFOSR DURINT program.
11:39AM J15.00003 A quantum algorithm for finding the modal value 1, MARK COFFEY 2, ZACHARY PREZKIUTA, Colorado School of Mines — We present a quantum algorithm for finding the most often occurring (or modal) value of a data set. We thereby supplement other algorithms that can determine the mean value or similar quantities. Our algorithm [1] requires the combined use of quantum counting and extended quantum search, and gives a quadratic speedup over the classical situation. For a data list of N elements, each entry an integer in the range [1,d], our method requires O(d N^{1/2}) oracle calls, and further complexity results are described. [1] to appear in Quantum Information Processing.

1 This work was partially supported by Air Force contract number FA8750-06-1-0001.

2 Department of Physics

11:51AM J15.00004 A Many Body Eigenvalue Problem for Quantum Computation 1, SELMAN HERSHFIELD, University of Florida — A one dimensional many body Hamiltonian is presented whose eigenvalues are related to the order of G_N. This is the same order of G_N used to decode the RSA algorithm. For some values of N the Hamiltonian is a noninteracting fermion problem. For other values of N the Hamiltonian is a quantum impurity problem with fermions interacting with a spin-like object. However, the generic case has fermions or spins interacting with higher order interactions beyond two body interactions. Because this is a mapping between two different classes of problems, one of interest in quantum computing and the other a more traditional condensed matter physics Hamiltonian, we will show (i) how knowledge of the order of G_N can be used to solve some novel one dimensional strongly correlated problems and (ii) how numerical techniques, particularly for quantum impurity limit, can be used to find the order of G_N.

1 We thank NSA (grant MOD713106A) for financial support.

12:03PM J15.00005 Generating Pseudo-Random Quantum States with Cluster Computation 3, WINTON G. BROWN, Dartmouth College, YAAKOV S. WEINSTEIN, The MITRE Corporation, LORENZA VIOLA, Dartmouth College — We revisit existing algorithms for generating pseudo-random pure quantum states in the light of cluster-state quantum computation. Reformulation of previous network-based algorithms in terms of appropriate measurement patterns suggests a (nearly) optimal distribution of local single-qubit gates, which results in a significant improvement in the asymptotic rate of purity decay. Surprisingly, this distribution is not the one corresponding to arbitrary random single qubit rotations. We find that the rate at which the expected purity approaches the prediction based on the Haar measure is asymptotically constant with respect to the number of logical qubits. Connectivity of the underlying qubit coupling topology as well as the occurrence of saturation and cut-off effects are analyzed.

3 Partially supported from Constance and Walter Burke through their Special Projects Fund in Quantum Information Science.

12:15PM J15.00006 Ground States as Resources for Universal Measurement-Based Quantum Computing 1, ADAM G. D’SOUZA, DAVID L. FEDER, University of Calgary — Measurement-based quantum computation (MBQC) requires a massively entangled resource state (such as a cluster state) as input. Experimental efforts towards generating such states have typically focused on performing global entangling operations on uncorrelated qubits. As the states that result from this type of procedure are not generally ground states, they are very sensitive to decoherence effects. A more robust resource would be one that is in fact a ground state of some Hamiltonian that exhibits a reasonably large energy gap between the ground state and the various excited states. We will discuss the possibility of finding simple two-body spin Hamiltonians whose ground states are equivalent to resource states for MBQC under stochastic protocols comprised solely of local operations and classical communication.

1 This work was supported by funding from NSERC and iCORE.

12:27PM J15.00007 Quantum Non-demolition measurements of single spins in semiconductors 3, MOHAN SAROVAR, KEVIN YOUNG, University of California, Berkeley, THOMAS SCHENKEL, Lawrence Berkeley National Laboratory, K. BIRGITTA WHALEY, University of California, Berkeley — For the development of large-scale quantum computers, electron spin-encoded qubits in solid-state are appealing because of their favorable decoherence time scales, high potential for scalability, and many handles for precision control. However, an additional requirement that is traditionally challenging in the solid-state is a capacity for high-fidelity qubit readout. We propose a scheme for measuring the state of a single donor electron spin using a field-effect transistor induced two-dimensional electron gas and electrically detected magnetic resonance techniques. The scheme is facilitated by hyperfine coupling to the donor nucleus. We analyze the potential sensitivity and outline experimental requirements. Our measurement provides a single-shot, projective, and effectively quantum non-demolition measurement of an electron spin-encoded qubit state.

3 We thank NSA (grant MOD713106A) for financial support.

12:39PM J15.00008 Adiabatic optical two-qubit operation with electron spins in separate quantum dots 1, SEMION SAIKIN, University of California, San Diego, LA Jolla, CA 92093, CLIVE EMARY, Institut fur Theoretische Physik, TU Berlin, D-10623 Berlin, Germany, DUNCAN STEEL, University of Michigan, Ann Arbor, MI 48109, LU SHAM, University of California, San Diego, La Jolla, CA 92093 — We develop an adiabatic scheme to control the entanglement of two electron spins localized in separate InAs/GaAs quantum dots via the Coulomb interaction between two negative trions optically excited in the different dots. The scheme gives a unitary operation in the spin subspace and can be used as a two-qubit gate for quantum information processing. The slowly-varying adiabatic pulses drive the system in a such way that effects of pulse imperfections and relaxation of the trion states are minimized. For spin dynamics we provide an exact numerical solution that accounts for dissipation and analyze the essential processes within a “dressed state” model. Our calculations for vertically-stacked quantum dots show that for a broad range of dot parameters a two-spin state can be prepared coherently from an initially polarized state by four optical fields with the pulse duration \Delta t \sim 1 ns.

1 This work was supported by ARO/NSA-LPS.

12:51PM J15.00009 Universal sets of quantum gates based on geometric phases 1, YU SHI, Fudan University, QIAN NIU, University of Texas at Austin — We rigorously study adiabatic and nonadiabatic geometric phases of two Heisenberg-coupled identical spins in a rotating magnetic field. The geometric phase of the total system is still a solid angle, and is independent of random Heisenberg coupling constant. The adiabatic geometric phase is also independent of the magnetic field rotating speed. Using this result, for both adiabatic and nonadiabatic cases, we explicitly and exactly construct novel robust dynamic-geometric-hybrid two-qubit square root of swap and controlled-NOT gates, as well as purely geometric single qubit gates, including \pi/8 and Hadamard gates, thus presenting a complete scheme of robust universal quantum computing. This scheme can be implemented in NMR, quantum dots and cold atoms.
effect. Several different conditions for existence of infinite hitting time are proven by analyzing the analytical structure of the formula for the infinite hitting that in the two limits of the measurement rate going to 0 or infinity the hitting time diverges, where the second limit is representative of the quantum Zeno and printed photodiode.

or 2D arrays of photodiodes can be printed onto diverse materials. Besides the dramatically reduced production costs for printed photodiodes, the presented modulation technique allows us to achieve a high signal to noise ratio even for high particle speeds. Combining our technique with a cell sorting mechanism would allow for on-the-chip characterization and sorting of untagged cells.

Physics and Astronomy, U. of Basel, P. STAMP, Dept. Physics and Astronomy, U. of British Columbia — Polyoxometalates (POMs) are discrete fragments of metal oxides, clusters of regular MOₙ polyhedra. POMs show a remarkable flexibility in composition, structure and charge state, and thus can be designed according to specific electric and magnetic needs. The two localized spins with S = 1/2 on the V atoms in [PMo₁₂O₄₀(V₂O₃)₈]⁶⁺ can be coupled through the delocalized electrons of the central core. This system was recently used for a theoretical scheme involving two-qubit gates and readout: the electrical manipulation of the molecular redox potential changes the charge of the core and thus the effective magnetic exchange between the qubits. Polyoxometalates can encapsulate magnetic ions, protecting them by a diamagnetic shell of controlled geometry. A great potential of POMs as spin qubits is that they can be constructed using only even elements, such as O, W, Mo and/or Si. Thus, there is a high abundance of polyoxometalate molecules without any nuclear spin, which could result in unusually low decoherence rates. There is currently an effort involving highly anisotropic, high magnetic moment, lanthanide@polyoxometalate molecules acting as spin qubits.

1:51PM J15.00014 ABSTRACT WITHDRAWN —

Tuesday, March 11, 2008 11:15AM - 2:15PM –

11:15AM J16.00001 Direct-Print Organic Photonics for Biodetection Chips — MAX SONNLEITNER, BIOIDENT Technologies Inc. — The development of commercial portable Biodetection applications based on optical detection is hindered by the lack of imaging systems that can be directly integrated into the chip itself. Currently, fluorescence/luminescence signals are read out with power-hungry, bulky and expensive off-chip imaging systems, like CCD cameras or photomultiplier tubes. Here we present an enabling technology that for the first time allows cheap and easy integration of imaging systems directly into disposable Biodetection systems. Our technology is based on organic semiconductor materials that can be processed in liquid form by inkjet and screen printing, in a process much faster and cheaper than the complicated fabrication of silicon-based imaging sensors. Organic photodiodes can be printed on various substrate materials like plastic foil or glass or directly onto Biochip systems. The ultra thin photodiodes with an overall thickness of only 300 to 500 nm show quantum efficiencies better than 0.5 and linear light-response over 6 orders of magnitude. The pixel size can range from 50 to over 1000 μm and inkjet fabrication allows tailoring the sensor layout to the needs of the specific application. Single photodiodes, photodiode line-arrays or 2D arrays of photodiodes can be printed onto diverse materials. Besides the dramatically reduced production costs for printed photodiodes, the presented readout architecture allows detection of e.g. chemiluminescence signals with highest sensitivities and minimum crosstalk due to the close proximity of sample and printed photodiode.

11:51AM J16.00002 On-the-flow differentiation between cells based on native fluorescence spectroscopy on a chip — MARKUS BECK, MICHAEL BASSLER, PETER KIESEL, NOBLE M. JOHNSON, OLIVER SCHMIDT, Palo Alto Research Center, 3333 Coyote Hill Rd, Palo Alto, CA 94034 — Native fluorescence spectroscopy is a promising approach for the detection of pathogens without specific binding or tagging of the analyte. The distinction between different species is possible with (multi-color) UV excitation together with the detection of several spectral bands. We have developed a compact platform that combines a microfluidic quartz channel with chip-size wavelength-selective detection of the fluorescence from particles traversing the channel. The interaction between the UV excitation light and the analyte is enhanced by anti-resonantly guiding the light within. We have recorded the intrinsic fluorescence of single cells (e.g. yeast, e-coli, and BT) passing the detection area. Knowing the particle speed and the physical dimensions of the observation window, we are able to determine particle positions with microscopic (∼10 microns) resolution. A special modulation technique allows us to achieve a high signal to noise ratio even for high particle speeds. Combining our technique with a cell sorting mechanism would allow for on-chip characterization and sorting of untagged cells.
12:03PM J16.00003 Toward directed evolution of unicellular organisms for efficient hydrogen production1 | DAVID LIAO, CALEB HOWE, CECILIA MULDOON, PETER GALAJDA, KEITH MORTON, PRINCETON UNIVERSITY — To provide an energy resource alternative to fossil fuels, photosynthetic organisms must increase their energy conversion efficiency. The green algae C. reinhardtii stores light energy in hydrogen gas at 0.1% efficiency, less than the 10% required to compete with established fuels. This work combines hydrogen sensing in liquid culture with micro habitat patch (MHP) chips for directing hydrogen-producing organisms to evolve improved energy conversion efficiency. A MHP chip contains 87 mm x 1 mm x 100 mm interconnected chambers. By measuring hydrogen output from different chambers, we will select those with greater hydrogen production. We microfabricated chips from poly(dimethylsiloxane). Color changes in fluorescence micrographs confirm that 254 nm radiation kills algae in MHPs, liberating nutrients and space for exploitation by adjacent populations. We demonstrated colorimetric detection of hydrogen gas production at a rate of 10^{-11} mol H2 mL^{-1} s^{-1} using tungsten film on sub-ML liquid cultures of C. reinhardtii during 2-hrs. of fermentation in darkness.

1Supported by DARPA grant W911NF-05-1-0392

12:15PM J16.00004 Toward on-chip directed evolution of unicellular organisms for efficient hydrogen production1 | DAVID LIAO, CALEB HOWE, CECILIA MULDOON, PETER GALAJDA, KEITH MORTON, PRINCETON UNIVERSITY — To provide an energy resource alternative to fossil fuels, photosynthetic organisms must increase their energy conversion efficiency. The green algae C. reinhardtii stores light energy in hydrogen gas at 0.1% efficiency, less than the 10% required to compete with established fuels. This work combines hydrogen sensing in liquid culture with micro habitat patch (MHP) chips for directing hydrogen-producing organisms to evolve improved energy conversion efficiency. A MHP chip contains 87 mm x 1 mm x 100 mm interconnected chambers. By measuring hydrogen output from different chambers, we will select those with greater hydrogen production. We microfabricated chips from poly(dimethylsiloxane). Color changes in fluorescence micrographs confirm that 254 nm radiation kills algae in MHPs, liberating nutrients and space for exploitation by adjacent populations. We demonstrated colorimetric detection of hydrogen gas production at a rate of 10^{-11} mol H2 mL^{-1} s^{-1} using tungsten film on sub-ML liquid cultures of C. reinhardtii during 2-hrs. of fermentation in darkness.

12:27PM J16.00005 Rapid Detection of Microorganisms—State of Art and Future Directions | GEORGE HONG, MILLIPORE CORPORATION — For the last several decades, nutrient-based culture growth methods have been accepted as the standard for microorganism detection and identification. However, since the discovery of nucleic acids and molecular breakthrough technologies such as restriction enzymes and polymerase chain reactions, the detection and identification of microorganisms have advanced to culture-independent methods that fall under the category of rapid microbial detections. Here, we present an overview of major rapid microbial detection technologies. These technologies include both amplification and non-amplification based methods for the detection and identification of target microorganisms. The technologies described can be applied to detecting a wide variety of microorganisms, including bacteria, viruses, mycoplasma, and fungi and have the potential sensitivity to detect a single microorganism. Also in this presentation, we will present examples of real-life applications as well as future challenges for the advancement of the field of rapid microbiology.

1:03PM J16.00006 Guidance and detection of neuronal cells using Si nanomembranes1 | CRISTIAN STAI, W.IDA ENG, HYUK JU RYU, DON E. SAVAGE, YU HUANG, SOOKIN NAM, JUSTIN WILLIAMS, ERIK DENT, MAX G. LAGALLY, SUSAN N. COPPERSMITH, MADISON — "Lab-on-a-chip" microfluidic technology [1] has emerged as a powerful tool for studying biological systems. Unlike standard micro-scale systems used for decades, microfluidics allows the micro-environment of a neuronal cell culture to be finely regulated. The reduction in feature sizes gives control over fluid phenomena such as laminar flow, shear stresses, and velocity profiles. Here we present a new approach to lab-on-a-chip, using microfluidic systems with silicon nanomembrane-based microelectronics. We show that this technology permits rapid production of microchannels with a large variety of shapes/sizes, thereby allowing the exposure of neuronal cell cultures to multiple environments, both mechanical and chemical, simultaneously. In addition, these microfluidic channels can be easily integrated with silicon nanomembrane based electronics. [1] A.J.Blake, T.M.Pearce, N.S.Rao, S.M.Johnson and J.C. Williams, Lab Chip, 2007, 7, 842.

1Work supported by: DOE, NSF, NIH-NINDS

1:15PM J16.00007 Well-Oriented NanoWell Array Metrics for Digital NanoBioChip | HEAYEON LEE, BONGKUK LEE, TOMOKI KAWAI, THE INSTITUTE OF SCIENTIFIC AND INDUSTRIAL RESEARCH (ISIR-SANKEN), OSAKA UNIVERSITY — Recently many researchers have sought new paradigm for nanobiotech that can be miniaturized and integrated to produce intelligent systems in numerous biotechnology. We present a new approach to nanofabrication, utilizing nanowires with novel properties that can be used to detect and manipulate biological molecules. We fabricated arrays containing nanowires with different properties, such as those that release light or electrical signals in response to specific molecules. These arrays can be used to detect and manipulate biological molecules with high sensitivity and specificity.

1:27PM J16.00008 Magnetically Directed Cell Co-Localization for Cell-Cell Interaction Studies | EDWARD FELTON, DANIEL REICH, Dept. of Physics and Astronomy, Johns Hopkins University, CHRISTOPHER CHEN, Dept. of Bioengineering, University of Pennsylvania — The ability to create ordered patterns of cells has enabled new approaches to various areas of biological interest, such as tissue engineering, biosensing, and the study of interactions between cells. In this work, we apply forces to cells through binding with magnetic nanowires. The nanowires feature high remanent magnetization, allowing for effective manipulation in low-strength magnetic fields, and when used in conjunction with lithographically patterned materials based nanopatterning, self-assembly array to address challenging problem in nanobiotechnology. In this work, we present an overview of major rapid microbial detection technologies. These technologies include both amplification and non-amplification based methods for the detection and identification of target microorganisms. The technologies described can be applied to detecting a wide variety of microorganisms, including bacteria, viruses, mycoplasma, and fungi and have the potential sensitivity to detect a single microorganism. Also in this presentation, we will present examples of real-life applications as well as future challenges for the advancement of the field of rapid microbiology.

1:30PM J16.00009 Electromagnetic Sensors of Biological Motors1 | JIE FANG, K. RAJAPAKSHE, D. PAD-MARAJ, H. INFANTE, V. VAJRALA, G. MERCIER, W. WIDGER, W. WOSIK, J. MILLER — Biological motors operate on time scales that readily couple to oscillatory electric fields. Modest ac fields applied to cells in an aqueous medium lead to greatly enhanced fields across the plasma membrane or (at kHz frequencies) internal membranes. Membrane complexes thus contribute to both linear and nonlinear responses to sinusoidal fields. For example, activity of motors in mitochondria and (for chloroplasts) photosynthetic electron transport chains correlate with frequency-dependent second and third harmonics. Our electrode-based biosensors are scalable for micro- and nano-fluidic biochips. At low frequencies (less than 100Hz) we find it advantageous to use SQUIDs, which reduce contact effects and could lead to clinical applications.

1The authors acknowledge support by R21CA122153 from NHLBI & NCI, NIH, & from NSF, by the Welch Foundation (E-1221), and by TcSUH.
**1:15PM J16.00010** Single-molecule stochastic sensors for proteins using engineered nanopores\(^1\), \textsc{Liuviu Movileanu}, Syracuse University — We were able to design an unusual temperature-responsive pore-based nanostructure with a single movable elastin-like-polypeptide (ELP) loop. If a voltage bias was applied, the engineered pore exhibited transient current blockades, the nature of which depended on the length and sequence of the inserted ELP. These blockades are associated with the excursions of the ELP loop into the nanopore. At low temperatures, the ELP is fully expanded and blocks the pore completely, but reversibly. At high temperatures, the ELP is dehydrated and structurally collapsed, thus enabling a substantial ionic flow. Acidic binding sites comprised of negatively-charged aspartic acid residues, engineered within the pore lumen, produced dramatic changes in the functional properties of the nanopore, catalyzing the translocation of cationic polypeptides from one side of the membrane to the other. For example, when two electrostatic binding sites were introduced, at the entry and exit of the nanopore, both the rate constants of association and dissociation increased substantially, diminishing the free energy barrier for translocation.

\(^1\)This work is funded by Syracuse University start-up funds and the US National Science Foundation, Grant DMR-706517

**2:03PM J16.00011** Imaging Protein-Functionalized Quantum Dot Diffusion and Binding at Surfaces\(^1\), \textsc{Jack Rife, James Long, Lloyd Whitman}, Naval Research Laboratory — Understanding single biomolecule and nanoparticle interactions with surfaces at fluid-solid interfaces is a key to improving molecular transport and binding in many biotechnology applications. Biosensor sensitivity, for example, is typically limited by diffusion\(^2\) and non-specific binding to analytical surfaces. We have assembled a Total Internal Reflectance Fluorescence (TIRF) microscopy system with single-photon-sensitive cameras to image diffusion and binding of fluorescently-labeled biomolecules on surfaces under both static and laminar flow conditions. We have acquired movies (57 frames/s) of streptavidin-functionalized CdSe quantum dots (QDs) diffusing, transiently attaching, and permanently immobilizing on repulsive, hydrophilic silica surfaces. From the single-particle trajectories we have extracted diffusion coefficients and transient attachment lifetimes. The binding of protein-functionalized QDs to our nominally repulsive surfaces can be attributed to surface defects, adsorbates, and protein conformational changes. In flow, the QD elevation above the no-slip surface can be approximated, giving a picture of elevated transport between transient attachments and QD departures to and from the surface. \(^2\) Sheehan and Whitman, Nano Lett. 5, 803 (2005).

\(^1\)Supported by the DTRA, Joint Science and Technology Office

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**Tuesday, March 11, 2008 11:15AM - 2:15PM — Session J17 DBP DMP: Focus Session: General Biological Patterns** Morial Convention Center 209

**11:15AM J17.00001** Relating biophysical properties across scales: implications for early development and applications for tissue engineering\(^1\), \textsc{Gábor Forgács}, Department of Physics, University of Missouri, Columbia, MO, 65211 — A distinguishing feature of a multicellular system is that it operates at various scales and levels of organization. Genes set up the conditions for physical mechanisms to act, in particular to shape the developing organism and establish its material characteristics. As development continues the changes brought about by the physical processes lead to changes in gene expression. It is through this interplay that the organism acquires its final structure and composition. It is natural to assume that in this multi-scale process the smaller defines the larger. In case of biophysical properties, in particular, those at the subcellular and cellular level are expected to give rise to those at the tissue level and beyond. Indeed, the physical characteristics of tissues vary greatly in physical properties: blood is liquid, bone is solid. In between these extremes lie most of the organs and tissues with intermediate visco-elast properties. However, a blood cell is not the same as a liquid drop and a single bone-forming cell itself is not a solid. Little is known on how tissue and organ level properties are related to cell and subcellular properties. We introduce a novel combined theoretical-computational-experimental framework to address this question. The basis of our approach is a representation of a cell by a network of interacting `organelles` (i.e. modules) with cell-specific properties. Cells form tissues and eventually organs through interactions either directly with each other or through secreted substances. The experimental and theoretical inputs of the formalism are inseparable: it cannot even be set up without one or the other. The method can serve as the basis for “computational tissue engineering”\(^2\).

\(^1\)Supported by the National Science Foundation #0526854.

**11:51AM J17.00002** Dynamics and Mechanics of Zebrafish Embryonic Tissues. \textsc{Eva-Maria Schoetz}, R.D. Burdine, M.S. Steinberg, Princeton University, C.-P. Heisenberg, MPI-CBG, R.A. Foty, UMDNJ, F. Julicher, MPI-PKS — In early zebrafish embryonic development, complex flows of cell populations occur, which ultimately lead to the spatial organization of the three germ layers: Ectoderm, mesoderm and endoderm. Here, we study the material properties of these germ layer tissues which are important for their dynamics and spatial organization in the embryo. In general, tissues can be classified as inherently active complex fluids. However, here we present examples of observed tissue behavior, which can be described satisfactorily in terms of passive visco-elastic fluids. We determined the material properties of the germ layer tissues quantitatively and found that differences in their properties influence tissue interaction. Specifically, quantitative differences in tissue surface tension result in tissue immiscibility and cell sorting behavior analogous to that of ordinary immiscible liquids. Surface tensions were measured with a tissue surface tensiometer. Furthermore, by tracking individual cells in the developing zebrafish embryo, we found differences in the migratory behavior of the different tissue types, which are, to some extent, governed by their mechanical properties. Finally, we generated a 3D velocity flow profile describing the tissue movements during zebrafish embryonic organizer development.

**12:03PM J17.00003** Laser Hole-Drilling as a Probe of Morphogenetic Stresses in Embryonic Epithelia: Experimental Observations\(^1\), \textsc{Xiaoyan Ma, M. Shane Hutson}, Vanderbilt University — During the development of an organism, sheets of epithelial cells expand, contract and bend due to forces generated within the cell sheets. These forces can be probed by laser hole-drilling — a method borrowed from the analysis of residual stress in manufactured widgets — in which a laser microbeam ablates a single cell surface or the edge shared by adjacent cells. We have applied this method to the embryonic epithelia of GFP-labeled fruit fly (Drosophila) embryos. After ablation of one shared edge, we follow the recoil dynamics (strain relaxation) of adjacent cell edges (with time resolution down to 2 ms). The recoils show two distinct phases; and the initial recoil velocity can be consistently retrieved through a double-exponential fit. We observe a strong correlation between the initial recoil velocity and the orientation of the ablated cell edge. This correlation is particularly pronounced in embryos during late dorsal closure. Measuring orientation with respect to the long (anterior-posterior) axis of the embryo, both the recoil velocities and the distribution of cell edge orientations have sharp peaks near 30° and 150°. In early dorsal closure, the distribution of cell edge orientation has three much weaker peaks and the recoil velocities only show a weak maximum near 90°.

\(^1\)This work supported by NSF Grant 0545679.
12:15PM J17.00004 Laser Hole-Drilling as a Probe of Morphogenetic Stresses in Embryonic Epithelia: Finite Element Models, M. SHANE HUTSON, XIAOYAN MA, Vanderbilt University, JIM VELDHUIS, G. WAYNE BRODLAND, University of Waterloo — During the development of an organism, sheets of epithelial cells expand, contract and bend due to forces generated within the cell sheets. These forces can be probed by laser hole-drilling; however, the observed recoil dynamics (or strain relaxations) depend strongly on the local cellular geometry. To better understand this dependence and help interpret our experimental observations, we have conducted a series of laser hole-drilling simulations using cell-level finite element models. Even the simplest of these simulations (i.e. homotypic cell sheets with constant cell boundary tensions) produce a wide range of initial recoil velocities. The velocities are correlated with particular aspects of the local geometry — most notably the aspect ratio and orientation of cells adjacent to the ablated cell edge. These simulations also produce bi-phase recoils; however, the two phases are not as distinct as those observed experimentally. To more closely reproduce the experimental recoils, the cell edges must include an elastic component. We will discuss using such finite element models to inversely determine local stresses in an epithelial sheet from the observed strain relaxations after laser ablation.

12:27PM J17.00005 Forces driven by morphogenesis modulate Twist Expression to determine Anterior Mid-gut Differentiation in *Drosophila* embryos, EMMANUEL FARGE, MGDET, UMR168 CNRS, Institut Curie11 rue Pierre et Marie Curie, F-75005, Paris, France — By combining magnetic tweezers to *in vivo* laser ablation, we locally manipulate *Drosophila* embryonic tissues with physiologically relevant forces. We demonstrate that high level of Twist expression in the stromodeal primordium is mechanically induced in response to compression by the 60±20 nN force developed during germ-band extension (GBE). We find that this force triggers the junctional release and nuclear translocation of Armadillo involved in Twist mechanical induction in the stromodeum in a Src42A dependent way. Finally, stromodeal-specific RNAi-mediated silencing of Twist during compression impairs the differentiation of midgut cells, as revealed by strong defects in Dve expression and abnormal larval lethality. Thus, mechanical induction of Twist overexpression in stromodeal cells is necessary for subsequent midgut differentiation. In collaboration with Nicolas Desprat, Willy Supatto, and Philippe-Alexandre Pouille, MGDET, UMR168 CNRS, Institut Curie11 rue Pierre et Marie Curie, F-75005, Paris, France; and Emmanuel Beaugeapre, LOB, Ecole Polytechnique, CNRS and INSERM U 696, 91128 Palaiseau, France.

1:03PM J17.00006 Mechanical forces in the development of leaf venation networks, FRANCIS CORSON, AREZKI BOUDAOUD, MOKHTAR ADDA-BEDIA, Laboratoire de Physique Statistique, Ecole Normale Superieure, Paris, France — Leaf venation patterns, like leaf shapes, are extremely diverse, yet their local structure has been shown to satisfy a simple, universal property: the angles veins form at junctions are related to their diameters by a vectorial equation analogous to a force balance. This structure is the signature of a reorganization of vein networks during the development of leaves, a process we investigated numerically using a cell proliferation model. Provided that vein cells are given different mechanical properties, tensile forces develop along the veins during growth, causing the network to deform progressively. The statistics of the patterns obtained in these simulations are in good quantitative agreement with observations on leaves, supporting the notion that the local structure of leaf venation networks reflects a balance of mechanical forces.

1:15PM J17.00007 Pattern Formation in a Synthetic Multicellular System, TING LU, DAVID KARIG, RON WEISS, Princeton University — Pattern formation has been studied for a long history since the Turing’s proposal for a reaction-diffusion system and been found in numerous physical, chemical and biological examples. However, experimental study about pattern formation advances slowly. Here we present an artificial pattern formation system. By engineering cellular communication in bacteria E. Coli and plating these engineered cells onto a solid-phase agarose plate, we are able to program the pattern formation of this multicellular system. The pattern changes dramatically with different levels of an external inducer IPTG. A simple model is developed to explain the experimental results.

1:27PM J17.00008 A Model of R8 Cell Specification in the *Drosophila* Eye, MATTHEW PENNINGTON, DAVID LUBENSKY, University of Michigan — R8 photoreceptors are specified in a precise hexagonal pattern behind an advancing front as it traverses the eye imaginal disc during *Drosophila* development. In an attempt to better understand this patterning event, we have developed a mathematical model consisting of coupled differential equations on a lattice incorporating auto-activation, long-range activation, and short-range inhibition. The model is based on known elements of the regulatory gene network involved in patterning, and an analogy with discrete Nagumo systems is helpful in understanding its dynamics. We have developed analytic and numeric results for its behavior on a 1D lattice. Significantly, this model can reproduce patterns similar to those seen both in wild-type eye discs and in several mutant phenotypes. We argue that much of the model’s behavior is a consequence of the fact that self-activation is cell-autonomous; this behavior represents a novel mode of pattern formation distinct from classical ideas such as Turing patterns or morphogen-dependent positional information.

1:39PM J17.00009 Emergence of hyper-hexagonal patterns in orientation map models of reduced rotation symmetry, WOLFGANG KEIL, MICHAEL SCHNABEL, FRED WOLF, BCCN and MPIDS, Goettingen, Germany — Neurons in the primary visual cortex preferentially respond to visual stimuli of a particular orientation. These orientation preferences are arranged in aperiodic 2-D patterns, known as orientation preference maps (OPMs). Symmetry assumptions have been used successfully to derive a class of theoretical model which accounts for the emergence of aperiodic pinwheel-rich OPMs. Measurements revealed anisotropic coupling statistics in the underlying neural tissue, suggesting that the symmetry of models for the formation of orientation map is reduced from the previously assumed E(2)xO(2) to E(2). In dynamical models for OPMs with E(2)xO(2) symmetry interactions represented by quadratic terms cannot occur but may be present in models of reduced E(2) symmetry. Here, we present a general analysis of the impact of such interactions on the formation of OPMs. We demonstrate that near the onset of pattern formation only two basic types of quadratic interaction terms exist, introduce a general parametric representation of permissible quadratic interactions near pattern formation onset, and derive the most general amplitude equations describing pattern selection in models incorporating quadratic interactions. We study the impact of such interactions on the spatial structure of OPMs, by incorporating them into a Swift-Hohenberg-model of OPM formation.

1:51PM J17.00010 Dynamics of Gas Exchange through the Fractal Architecture of the Human Lung, Modeled as an Exactly Solvable Hierarchical Tree, MICHAEL MAYO, PETER PFEIFER, Department of Physics, University of Missouri, Columbia, MO, 65211, STEFAN GHEORGHIU, Center for Complexity Studies, Alleea Parva 5, Bucharest 061942, Romania — The acinar airways lie at the periphery of the human lung and are responsible for the transfer of oxygen from air to the blood during respiration. This transfer occurs by the diffusion-reaction of oxygen over the irregular surface of the alveolar membranes lining the acinar airways. We present an exactly solvable diffusion-reaction model on a hierarchically branched tree, allowing a quantitative prediction of the oxygen current over the entire system of acinar airways responsible for the gas exchange. We discuss the effect of diffusion screening, which is strongly coupled to oxygen transport in the human lung. We show that the oxygen current is insensitive to a loss of permeability of the alveolar membranes over a wide range of permeabilities, similar to in a constant-current source in an electric network. Such fault tolerance has been observed in other treatments of the gas exchange in the lung and is obtained here as a fully analytical result.
2:03PM J17.00011 Evolution of Optimum Foraging Distributions in Two Dimensions, NATHAN DEES, SONYA BAHAR, FRANK MOSS, University of Missouri - St. Louis — In the pursuit of optimally efficient foraging, preferred distributions of movement characteristics have been shown to exist for many types of animals and environments. Specifically, planktonic organisms such as *Daphnia* use exponential distributions of turning angles, $\alpha$, in a “*hop, pause, turn by angle $\alpha$, hop…*” random walk-type sequence of movement when traversing experimentally prepared feeding solutions consisting of freeze dried *Spiroliana* and water. We investigate the evolution of such random walks in a two-dimensional foraging model. In this model, agents traverse a feeding patch of finite size and for a finite amount of time using hop lengths and turning angles chosen randomly from inherited distributions. Distributions evolve as the choices made by the most efficient forager of one generation influence the distributions available to the succeeding generation. Preliminary results show that initially uniform turning angle distributions evolve to explicit exponential distributions after thousands of generations, consistent with the experimental observations described above.

Tuesday, March 11, 2008 11:15AM-1:03PM
Session J18 DPOLY: Frank J. Padden Award Symposium Morial Convention Center 210

11:15AM J18.00001 Use DNA solutions to model polymer entanglement in flow: simultaneous rheometric and particle-tracking velocimetric measurements, POUYAN BOUKANY, SHI-QING WANG, Department of Polymer Science, University of Akron — Entangled aqueous DNA solutions are ideal as a model system to examine nonlinear flow features including stress overshoot in startup shear and shear thinning phenomenon. These soft systems can be strongly entangled with 60 entanglement points per chain and a terminal relaxation time as long as 1000 s at 1 % concentration [1-2]. They allow a comparison between the steady state attained with a startup shear and that attained through an “infinitely” slow ramping up of the applied shear rate. Indeed, startup shear in the nonlinear (stress plateau) region causes the DNA solutions to yield inhomogeneously, resulting in persistent shear banding. However, the slowly ramped-up shear into the same final rate as applied in startup shear allowed the solutions to avoid shear inhomogeneity. Thus, we demonstrated that it is possible for the final steady states to be different depending on how an entangled system is brought into the same final experimental condition. This result implies that it is ill-defined to pursue conventional constitutive relationship in flow of entangled polymers.


11:27AM J18.00002 Membrane-Enhanced Surface Acoustic Wave Analysis of Polymer Brushes, DAVID A. BRASS, KENNETH R. SHULL, Northwestern University — We show that detailed structural information about polymer brushes can be obtained from a simple membrane inflation technique in conjunction with a quartz crystal resonator. The sensitivity of these quartz crystal resonators is determined by the propagation of acoustic shear waves through the materials that are placed in contact with the oscillating crystal. Coupling of the shear acoustic waves into the membrane is strongly affected by the thickness of the brush layer, which is in turn affected by specific interactions between the polymer brush and the substrate with which it is brought into contact. The mechanical resonance of the quartz crystal is affected by these brush parameters, and we refer to the accompanying analysis of this resonance as ‘membrane-enhanced surface acoustic wave analysis’. The analysis combines self consistent mean field theory of the polymer brush with the relevant theories of acoustic wave propagation. The model has been tested experimentally with grafted poly(ethylene glycol) brushes in contact with thermoplastic elastomer membranes. We also show how the technique can be used to quantify the strength of specific interactions between the electrode surface of the quartz resonator and functional groups placed at the ends of the PEG brushes.

11:39AM J18.00003 Advances in Organic Single-Crystal Transistors, ALEJANDRO L. BRISENO, Department of Chemistry, University of Washington, ZHENAN BAO, Department of Chemical Engineering, Stanford University, YOUNAN XIA, Department of Chemistry, SAMSON A. JENEKHE, Department of Chemical Engineering, University of Washington — Organic semiconductors, including conjugated small molecules and polymers, constitute next-generation materials for displays, circuits, and a vast array of other electronic applications. The performances of organic single-crystal transistors have recently surpassed the performance levels of amorphous silicon devices. Despite the high mobilities of single-crystal devices, there are many factors limiting their applications. Currently, single crystals are handpicked and made into an individual device. Another challenge is to achieve control of crystallinity in polymer nanostructures. There is a need to explore nanowires as solution-processable materials because of the cost-effective aspect in fabricating devices. Therefore, in order to meet the requirements for fabricating practical devices, we have resolved the aforementioned issues by patterning organic single-crystal transistors and polymers. We have developed solution-phase methods for preparing organic single-crystal nanowires from p- and n-type semiconductors and highly oriented nanowires from polymer semiconductors. Furthermore, we have realized high-performance transistors and demonstrated the first all-polymer complementary circuit.

11:51AM J18.00004 Effect of lithium ion distribution on conductivity of block copolymer electrolytes, ENRIQUE GOMEZ, NITASH BALSARA, University of California, Berkeley — Energy-filtered transmission electron microscopy (EFTEM) was used to determine the distribution of lithium ions in mixtures of bis(trifluoromethane)sulfonimide lithium salt and symmetric poly(styrene-oxide) copolymers (PS-PEO). EFTEM results show that the salt is increasingly localized to the middle of the PEO lamellae as the molecular weight of the copolymers is increased. Computer simulations by Borodin and Smith (Macromolecules, 1998, 31, 8396) demonstrate that coordination between lithium ions and PEO chains is diminished for chains that are stretched. Local stretching in block copolymers is modeled using self-consistent field theory (SCFT). Good agreement between EFTEM and SCFT is obtained by postulating a linear relationship between local chain stretching and lithium ion concentration. AC impedance spectroscopy experiments show an increase in the conductivity of PS-PEO/salt mixtures with increasing molecular weight of PS-PEO. The EFTEM/SCFT results suggest that the increase in ionic conductivity with increasing molecular weight is due to segregation of the lithium salt away from PS/PEO interfaces where segmental motion is retarded due to connectivity to slow-moving PS chains. These results may aid in developing all-solid state rechargeable lithium batteries with PS-PEO serving as a dry electrolyte.

12:03PM J18.00005 Self-assembly of metal–polymer analogues of amphiphilic triblock copolymers, ZHIHONG NIE, DANIELE FAVA, EUGENIA KUMACHEVA, SHAN ZOU, GILBERT WALKER, Department of Chemistry, University of Toronto, Canada, MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina, USA, EUGENIA KUMACHEVA TEAM, SHAN ZOU, GILBERT C. WALKER COLLABORATION, MICHAEL RUBINSTEIN COLLABORATION — We proposed a block copolymer approach to the self-assembly of inorganic nanorods terminated with polymer molecules at both ends. We organized metal nanorods in structures with varying geometries by using a striking analogy between amphiphilic ABA triblock copolymers and the hydrophilic nanorods tethered with hydrophobic polymer chains at both ends. The self-assembly was tunable and reversible and it was achieved solely by changing the solvent quality for the constituent blocks. The distance between adjacent nanorods along the self-assembled structures is determined by varying the composition of mixture solvents or the molecular weight of polymer blocks, which allows us precisely control the plasmonic band of self-assembled structures. A systematic study of the self-assembly as a function of solvent composition and the molecular weight of the polymer blocks allowed us to construct a diagram that maps the assembled structures. This approach provides a new route to the organization of anisotropic nanoparticles by using the strategies that are established for the self-assembly of block copolymers.
12:15PM J18.00006 Rod-Coil Block Copolymer Self-Assembly in Thin Films, B.D. OLSEN, University of California Berkeley, V. GANESAN, University of Texas Austin, R.A. SEGALMAN, University of California Berkeley — The phase behavior of rod-coil block copolymers differs from that of traditional block copolymers due to the interplay between liquid crystallinity of the rod blocks and microphase separation of the rods and coils. A universal phase diagram for rod-coil diblock copolymers is prepared using experimental measurements of both the rod aligning interaction and the rod-coil repulsive interaction to transform the temperature-dependent phase transitions of a model-rod coil system into dimensionless parameter space. The rod aligning interaction, parameterized by the Maier-Saupe parameter, may be estimated from the dependence of the nematic-isotropic transition temperature on the molecular weight of the rod homopolymer. The rod-coil interaction, parameterized by the Flory-Huggins parameter, is calculated from the temperature-dependent interfacial segregation of block copolymer to a rod/coil homopolymer interface. The Flory-Huggins parameter is extracted by using it as a fitting parameter in self-consistent field theory to match simulated block copolymer surface excesses to experimental values.

12:27PM J18.00007 Why nanoconfinement may lead to the development of polymer glasses that do not physically age, RODNEY PRIESTLEY, LINDA BROADBELT, JOHN TORKELSON, Department of Chemical and Biological Engineering, Northwestern University — With the advent of nanotechnology, polymers will be used at increasingly smaller length scales, i.e., the nanoscale. Recently, it has been shown that nanoconfined polymers can exhibit astounding changes in glassy-state properties relative to bulk. Physical aging, i.e., the change in properties as a function of annealing time below the glass transition temperature, determines the end-use properties of polymer glasses. How nanoconfinement impacts aging has emerged as a key technological and scientific question. Conventional techniques for monitoring aging of bulk polymers are incapable of doing so for nanoconfined polymers. Here, we present work in which we have developed fluorescence methods to monitor aging in thin polymer films. More importantly, our technique allows for the monitoring of aging at specific locations in films near interfaces. Our work indicates that nanoconfinement and interfacial effects strongly alter aging and that the development of polymer glasses that do not physically age may be possible.

12:39PM J18.00008 Ionic Complexation Enhanced Block Copolymer Alignment with an Electric Field, JIA-YU WANG, THOMAS P. RUSSELL, University of Massachusetts, Amherst — Alignment of microdomains in block copolymer (BCP) films by an electric field offers the possibility of fabricating ordered nanostructures that are used as templates, scaffolds and masks. In polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) copolymer films, the formation of lithium-PMMA complexes, as a result of the added lithium salts, markedly enhanced the alignment of BCP microdomains under an electric field, due to the increased dielectric contrast and the weakened surface interactions which reduced the critical field strength. The formation of lithium-PMMA complexes also increases the segmental interaction, parameterized by the Maier-Saupe parameter, may be estimated from the dependence of the nematic-isotropic transition temperature on the molecular weight of the rod homopolymer. The rod-coil interaction, parameterized by the Flory-Huggins parameter, is calculated from the temperature-dependent interfacial segregation of block copolymer to a rod/coil homopolymer interface. The Flory-Huggins parameter is extracted by using it as a fitting parameter in self-consistent field theory to match simulated block copolymer surface excesses to experimental values.

12:51PM J18.00009 Polymer Surface Diffusion as a Function of Molecular Weight, JANET WONG, STEVE GRANICK, Dept. Materials Science and Engineering, University of Illinois at Urbana-Champaign — This talk describes the first measurements to elucidate polymer surface diffusion over the full range of surface concentration and as a function of molecular weight. The model system, polystyrene adsorbed onto mica and quartz from chloroform, was selected to allow molecular weight (M) to vary by more than 2 orders of magnitude and the surface coverage to vary by more than 3 orders of magnitude. Spatially-resolved measurements of surface translational diffusion (D_s) were made using fluorescence correlation spectroscopy (FCS), which is a single-molecule technique. The value of D_s was found to scale as a power-law in M. Remarkably, the absolute value of the power-law was -1 for mica and the most homogeneous quartz surfaces, -3/2 for less homogeneous quartz surfaces, and never took intermediate values. Explanations remain speculative but appear to involve the dominance of Rouse and reptation diffusion mechanisms, respectively. In the latter case, curvilinear motion is guided not by entanglement with other chains but instead by patchiness (topographical and chemical) of the surface adsorption sites.

Tuesday, March 11, 2008 11:15AM - 2:15PM –
Session J19 FD: Focus Session: How to Develop an Education Component for an NSF Proposal
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11:15AM J19.00001 How to develop an education component for an NSF proposal, RANDY RUCHTI, University of Notre Dame — NSF has two merit criteria that must be satisfied for a proposal to be successfully funded: Intellectual Merit and Broader Impact. The development and presentation of a quality broader impact program represents a challenge for many researchers. One option is an education component and there are many possible approaches: in formal or informal education; in engagement of traditional, non-traditional or underrepresented participants; in coverage over a variety of age groups; and in scope. This presentation explores such issues and is intended to elicit discussion.

1Work supported in part by the National Science Foundation.

11:51AM J19.00002 Preparing Scientists for Scientific Careers: Broader Impacts from an NSF CAREER Award, ALFRED CROSBY, University of Massachusetts Amherst — The scientific focus of my NSF CAREER Award is the impact of patterns, topographical and surface chemical in design, on the adhesion of soft polymer interfaces. Although this topic has provided a strong foundation for the mentoring and training of graduate students, the primary broader impacts of my award have focused on the development of “soft” skills in graduate and post-doctoral researchers in STEM disciplines. I have developed a course on “Scientific and Engineering Management,” which provides an open forum for students to explore the skills that, in many ways, define successful careers for many scientists. Topics include: leadership, proposal writing, group management, communication in diverse environments, and ethics. In this presentation, I highlight the primary phases of this program, how it meshes with scientific goals, and general statements about the mission of education outreach within STEM disciplines.

12:03PM J19.00003 Educational Component of an NSF-CAREER Award on State Variables in Dense Granular Materials, KAREN DANIELS, North Carolina State University — I will discuss the design and goals of the educational component of an NSF-CAREER award whose research mission centers around experiments on granular materials. Two of the activities primarily involve undergraduates: providing laboratory research opportunities in support of the scientific goals of the project, and developing and disseminating an introductory seminar course on nonlinear nonequilibrium systems. In addition, the students from both the course and the laboratory will develop, in collaboration with NC State’s Science House, hands-on outreach activities for use with local school/youth groups.
12:15PM J19.00004 Education component of NSF awards – what can be done and where can we make a difference, ALESSANDRA LANZARA, University California, Berkeley — The education component of the NSF awards is often neglected or considered a minor component of the research. In this talk I will share my personal view of the importance of this component. In particular I will provide few examples of situation I have encountered in the past few years as NSF career awardees and will discuss what in my opinion are the aspects one should focus on to make a difference.

12:27PM J19.00005 Introducing Change in Undergraduate Education (Easy Steps for Junior Faculty), ERIC HUDSON, MIT — Bringing change to the undergraduate curriculum – for example, as new faculty might consider proposing for the Faculty (including junior faculty) could make to well established courses while avoiding the difficulties often associated with change. In this talk I will describe TEAL (technology enabled active learning), a major reform to the introductory physics sequence for non-majors at MIT. I will then focus on a few aspects of the course, such as the use of in-class feedback and real world problems. These relatively small changes (in terms of expense and effort) have been very beneficial, and point to a variety of improvements which faculty (including junior faculty) could make to well established courses while avoiding the difficulties often associated with change.

12:39PM J19.00006 Integration of Education and Research: proposed and completed activities, VERA SMOLYANINOVA, Towson University — In my presentation I will share my ideas of integrating education and research in a setting of an undergraduate institution. The proposed educational component of my CAREER proposal will be compared to what has been completed taking into account evolving needs and goals of our department, college and university. Organization of undergraduate research, curriculum development, and outreach activities will be discussed. Future plans will be introduced.

12:51PM J19.00007 Caltech Classroom Connection: An Outreach Partnership Program Between Caltech Scientists and K-12 Teachers, JAMES MALONEY, JENNIFER FRANCK, TARA GOMEZ, CHRISTINA SMOLKE, JOHN KEITH, California Institute of Technology — The Caltech Classroom Connection (CCC) is a volunteer outreach program whose goal is to supplement science, math and engineering education in local K-12 classrooms through individual scientist-teacher partnerships. Caltech graduate students, postdocs, staff and faculty volunteers are paired with teachers to develop a mutually beneficial and sustainable partnership. Targeted schools include the Pasadena Unified School District in which 76% of the student demographic consists of Hispanic and African American students, historically underrepresented in science, math and engineering careers. Student surveys are being developed to follow trends in science attitudes and science appreciation after interaction with a Caltech volunteer throughout the school year. The students are also affected by the increase in science awareness and confidence of the teacher, especially at the elementary level. We will present the program’s results over the past five years as well as future plans for improvement and expansion.

1:03PM J19.00008 Squishy Physics Field Trips, ERIC R. WEEKS, GIANGUIDO CIANCI, Emory University, PIOTR HABDAS, St. Joseph’s University — Our laboratory studies soft condensed matter, which means we investigate squishy materials such as foams, emulsions, and colloidal suspensions. These materials include common things such as peanut butter, toothpaste, mayonnaise, shampoo, and shaving cream. We have conducted several field trips for grade school students, where they come to our laboratory and play with squishy materials. They do both hands-on table-top projects and also look at samples with a microscope. We have also developed some of these activities into labs appropriate for first-year college students. Our first goal for these activities is to show students that science is fun, and the second goal is to get them intrigued by the idea that there are more phases than just solids, liquids, and gases.

1:15PM J19.00009 Moving Research into the Classroom with the Electron Microscopy Database, PAUL VOYLES, University of Wisconsin, Madison — Due to the strongly interdisciplinary nature of research in nanotechnology and materials, a course on transmission electron microscopy (TEM) must often serve student from a very broad range academic disciplines, level of background, and research interests. Someone in the class will want to learn about all the possible capabilities of the TEM, which span diffraction, spectroscopy, and imaging. Research students learn best from real-world examples, which are usually drawn from the research of the instructor, but very few instructors have the breadth of research and instrumentation needed to obtain high-quality examples of all the possible combinations of techniques and materials. I have therefore developed the Electron Microscopy Database (EMdb, http://tem.msa.e.wisc.edu/emdb/) as part of the education plan of my NSF CAREER project. The goal of the EMdb is to enable TEM teachers to easily exchange high-quality TEM example data and associated homework problems. This serves the NSF education goals of promoting excellence in research training and of bringing cutting-edge research into the classroom, and has significantly improved my own teaching.

1:27PM J19.00010 Research Experiences for Teachers: How professional development through directed research can revitalize your classroom teaching, SHELLY HYNES, Louisiana School for Math, Science and the Arts — Research Experiences for Teachers (RET) is an NSF-funded program that provides high school teachers with the opportunity to do research at select institutions across the country in a wide variety of fields. I performed research at two institutions under this program: The National Radio Astronomy Observatory in Green Bank, WV in 2006 and Baylor University in Waco, TX in 2007. My work at NRAO utilized IDL programming to analyze the nonlinearities in the signal processing components of the GBT (Green Bank Telescope). My research at Baylor University required me to write a program in Mathematica to analyze the frequency of pulsation of variable white dwarfs, data that was taken at the Paul and Jane Meyer Observatory in Clifton, TX. I will explain how I have incorporated both research experiences into my courses and how each of these experiences has refocused my teaching.

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Research supported via the NSF-RET program, NRAO, Associated Universities, Inc., Baylor University, and the Central Texas Astronomical Society.
Barrier Height on H-Terminated Si(100) Surface

In scanning tunneling microscopy (STM) measurements on semiconductor surfaces, tip-induced band bending (TIBB) occurs due to the applied high bias voltage, and influences the local electronic structures of the surface detected by STM and scanning tunneling spectroscopy (STS). Recently, Yoshida et al. have reported the effect of the TIBB on local tunneling barrier height (LBH) on Si(100) surfaces by light-modulated STS [1]. However, theoretical studies on the TIBB and LBH have not been performed yet on semiconductor surfaces. In this study, we have analyzed the TIBB and LBH on an H-terminated Si(100) surface theoretically using the boundary-matching scattering-state density functional method [2], which can calculate the electron states under applied bias voltages self-consistently. In particular, we focus on the bias voltage dependences of the TIBB and LBH, and show that measured data also confirm such quasi-one dimensional character with a very anisotropic band structure. The surface electronic density of states measured by tunneling spectroscopy is compared with theoretical calculations.

1 Supported by the Research Corporation Cottrell Scholar Award and NSF-CAREER-DMR0449899.

2:03PM J19.00013 Inciting High-School interest in physics,1 JIANDI ZHANG, Florida International University (FIU), Miami, FL 33199 — We report on our outreach effort on material-physics education program as one part of my NSF Career award project. This is a program incorporated with the NSF funded Physics Learning Center at FIU, focusing on the material physics enrichment both high school students and teachers. We particularly pay attention to minority students by taking the advantage of FIU’s composition and location. The program offers a special/session-style workshop, demonstrations, research lab touring, as well as summer research activities. The goal is to enrich teacher’s ability of instruction to their students and inspire students to pursue scientific careers. The detailed outreach activities will be discussed.

1 Supported by NSF DMR-0346826

Tuesday, March 11, 2008 11:15AM - 2:15PM —Session J20 DCMP: Focus Session: Electronic and Lattice Properties of Surfaces and Thin Films Morial Convention Center 212

11:15AM J20.00001 Atomic and Electronic structure of Fe2O3 films on MgO(111). K. PANDE, University of Wisconsin-Milwaukee, A. CELIK-AKTAS, M. GAJDARDZISKA-JOSIFOVSKA, M. WEINERT — Polar oxide surfaces have interesting properties due to the strong ionic character of the metal-oxide bonds and the layering of metal and oxygen planes parallel to the surface. In this first-principles study we investigate the effect of MgO(111) surface polarity on the structure of iron oxide films. The calculated energetics of different surface terminations on the unreconstructed MgO(111) surface suggest that the interface has a Mg-O-Fe stacking with no intermixing of O and Fe atoms at the interface. The magnetic ordering of Fe atoms both within the layers and between neighboring (bi)layers will be described. The calculated structural and electronic properties will be compared to the results of high-resolution transmission electron microscopy (HRTEM) and selective area diffraction (SAD) experiments of Fe2O3 films on MgO(111) surface.

11:27AM J20.00002 ABSTRACT WITHDRAWN

11:39AM J20.00003 The semiconducting surface of In0.53Se1.53, M. KLINKE, E. CAI, I. RODRIGUEZ, JIANDI ZHANG, Florida International University, R. MATZDORF, Univ. Kassel, Y. LOSOVYI, J. LUI, P.A. DOWBEN, Dept. of Physics and Astronomy and the Nebraska Center for Material and Nanoscience, L. MAKINISTIAN, Facultad de Ingeniería, Univ. Nacional de Entre Ríos, E.A. ALBANCESI, INTEC-CONICET, A. PETUKOV, South Dakota School of Mines, Dept. of Physics, YA. FIYALA, P. GALIY, Electronics Dept., Lviv National Univ. — The layered crystal In0.53Se1.53 is of growing interest because of its nano-scale two dimensional structure and interesting transport properties. We have studied both the lattice and electronic band structures of cleaved (001) surface of In0.53Se1.53. Both LEED and STM reveal a p(1x1) surface structure with quasi-one dimensional atomic chains. ARPES data also confirm such quasi-one dimensional character with a very anisotropic band structure. The surface electronic density of states measured by tunneling spectroscopy is compared with theoretical calculations.

1 NSF CHE-0415421

11:51AM J20.00004 Theoretical Study of Tip-Induced Band Bending and Local Tunneling Barrier Height on H-Terminated Si(100) Surface, HIDEOMI TOTSUKA, Nihon University, SATOSHI WATANABE, The University of Tokyo, CREST TEAM — In scanning tunneling microscopy (STM) measurements on semiconductor surfaces, tip-induced band bending (TIBB) occurs due to the applied high bias voltage, and influences the local electronic structures of the surface detected by STM and scanning tunneling spectroscopy (STS). Recently, Yoshida et al. have reported the effect of the TIBB on local tunneling barrier height (LBH) on Si(100) surfaces by light-modulated STS [1]. However, theoretical studies on the TIBB and LBH have not been performed yet on semiconductor surfaces. In this study, we have analyzed the TIBB and LBH on an H-terminated Si(100) surface theoretically using the boundary-matching scattering-state density functional method [2], which can calculate the electron states under applied bias voltages self-consistently. In particular, we focus on the bias voltage dependences of the TIBB and LBH, and show that measured LBHs can be basically understood as the sum of TIBB and intrinsic barrier height. [1] S. Yoshida, et al., e-J. Surf. Sci. Nanotech. 4, 192 (2006). [2] Y. Gohda et al., Phys. Rev. Lett. 85, 1750 (2000). [3] M. McEllistrem, et al., Phys. Rev. Lett. 70, 2471 (1993).
12:03PM J20.00005 Studies of the oxidized Cu(100) surface using positron annihilation induced Auger electron spectroscopy, W. MADDOX, N. G. FAZLEEV, M. P. NADESEILINGAM, A. H. WEISS, Department of Physics, University of Texas at Arlington — We discuss recent progress in studies of an oxidized Cu(100) single crystal subjected to vacuum annealing over a temperature range from 293K to 1073K using positron annihilation induced Auger electron spectroscopy (PAES). The PAES measurements show a large monotonous increase in the intensity of the positron annihilation induced Cu M2,3VV Auger peak as the sample is subjected to a series of isochronal anneals in vacuum up to annealing temperature 573 K. The intensity then decreases monotonically as the annealing temperature is increased to 873 K. Experimental PAES results are analyzed by performing calculations of positron surface states and annihilation probabilities of surface-trapped positrons with relevant core electrons taking into account the charge redistribution at the surface, surface reconstructions, and electron-positron correlations effects. The effects of oxygen adsorption and surface reconstruction on localization of positron surface state wave functions and annihilation characteristics are analyzed. Possible explanations are provided for the observed behavior of the intensity of positron annihilation induced Cu M2,3VV Auger peak with changes of the annealing temperature.

12:15PM J20.00006 Visualization of 2D subband states formed in Si(111)-β-√3x√3-Bi surface by STM, KATSUMI NAGAOKA, SHIN YAGINUMA, TADAAKI NAGAO, TOMONOBU NAKAYAMA, National Institute for Materials Science — We have investigated electronic subbands formed underneath of Si(111)-β-√3x√3-Bi (β-√3-Bi) surface by using STM. The β-√3-Bi surface is semiconducting, and the band gap is larger than that of bulk Si. In the dI/dV images, standing waves are found around defects, and the obtained energy dispersion is in good agreement with the free-electron-like model. Apparently, formation of a 2D electronic state is suggested. However, this standing wave is observed only on p-type, but not on n-type Si substrates, and consequently the 2D state is attributed to the subband formed in the depletion layer just below the β-√3-Bi surface. The subband formation is also consistent with the calculation of electronic states inside a potential-well caused by interfacial band bending.

12:27PM J20.00007 One-Dimensional Electronic Bands of Monatomic Cu Chains, PINGHENG ZHOU1, International Center for Theoretical Physics, Trieste, Italy, PAOLO MORAS, Istituto di Struttura Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy, LUISIA FERRARI, Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Roma, Italy, GUSTAV BIHLMAIER, STEFAN BLÜGEL, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany, CARLO CARBONE, Istituto di Struttura Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy — The electronic structure of an array of monatomic Cu chains grown on the Pt(997) surface has been examined by angle-resolved photoemission. The monatomic wires exhibit properties associated to 3d electron confinement in one-dimension. Along the wire direction the 3d bands states display a dispersive character, with periodicity in reciprocal space defined by the wire array geometry. These observations are compared and analyzed with ab initio calculations based the full potential linearized augmented plane wave method.

12:39PM J20.00008 Calculating work functions with density functional theory: the effect of finite temperature, surface alloying, and oxidation, THOMAS R. MATTSSON, DWIGHT R. JENNISON, Sandia National Laboratories, Albuquerque, NM 87185-1186, USA — The work functions for W, Cu, and Al are calculated using density functional theory (DFT). We go beyond the perfect lattice at zero Kelvin by employing molecular dynamics techniques. Effects of surface alloying and oxidation are also investigated. The effect of alloying and oxidation is, as expected, found to be significant, whereas the temperature dependence, although detectable, is small. Furthermore, the exchange-correlation density functional AM05 is compared to the results of LDA and PBE. The calculated work functions compare well to available experimental results. This work was supported by the LDRD office and the simulations were performed at the High Performance Computing facilities at Sandia National Laboratories, NM. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:51PM J20.00009 Longitudinal Phonon Resonance of the Cu(111) Surface, VASSE CHIS, BO HELLING, Department of Physics, Göttingen University, Sweden, MARCO BERNASCONI, GIORGIO BENDEK, Dipartimento di Scienze dei Materiali, Università Milano-Bicocca, Milano, Italy, J. PETER TOENNIES, Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — The electronic structure of an array of monatomic Cu chains grown on the Pt(997) surface has been examined by angle-resolved photoemission. The monatomic wires exhibit properties associated to 3d electron confinement in one-dimension. Along the wire direction the 3d bands states display a dispersive character, with periodicity in reciprocal space defined by the wire array geometry. These observations are compared and analyzed with ab initio calculations based the full potential linearized augmented plane wave method.

1:03PM J20.00010 Rashba-type spin-orbit splitting in ultrathin Bi films, G. BIHLMAIER, Inst. f. Festkörperforschung, FZ Juelich, Germany, YU. M. KOROTEEV, Inst. of Strength Physics and Materials Science, Tomsk, Russia, E.V. CHULKOV, Donostia International Physics Center, San Sebastian, Spain, S. BLÜGEL, Inst. f. Festkörperforschung, FZ Juelich, Germany — Due to their electronic similarity with graphene sheets, surfaces and thin films of the semimetal bismuth have recently received considerable interest. A systematic study of thin (1 – 6 bilayers) films in (111) and (110) orientation is presented, employing density functional theory calculations. Due to the different coordination of the surface atoms in these two cases, a large variation of the conducting properties of the films is found. The evolution of surface states is studied as a function of the film thickness and by comparison to thicker films and simulations of the semimetallic crystals. Interesting features arise from the strong spin-orbit effects in Bi and the resulting Rashba-type spin-splitting of the surface states. The spin-polarization of these states changes as these states transform into quantum well states at the Brillouin zone boundary. The results are compared with recent experimental results on Bi films on Si substrates.

1:15PM J20.00011 Lattice Dynamics of RuO2: Bulk and (110) Surface, KLAUS-PETER BOHNEN, ROLF HEID, Forschungszentrum Karlsruhe, IFP, OMAR DE LA PENA SEAMAN, Department of Applied Physics, CINVESTAV-Merida — Although RuO2 has been studied as a prototype catalyst for CO oxidation no careful study of the lattice dynamics for this material has been presented so far. Using modern ab-initio methods we obtain the phonon dispersion and the generalized density of states (GDOS). Inelastic neutron-scattering experiments allow for an experimental determination of the GDOS. In contrast to what is known from structural studies, we find that the local-density approximation gives a much better description of the phonon spectrum than the generalized gradient corrected form. This is also consistent with Raman measurements. Besides the bulk we have also studied the lattice dynamics for the (110) surface. Our calculations indicate an instability over a large range of the BZ. Unfortunately, no complete experimental phonon study of this surface has been carried out so far. Consequences for the structure of the (110) surface will be discussed.
1:27PM J20.00012 Simulation of four-probe measurement based on density-functional tight-binding method, ASAKO TERASAWA, TOMOFUMI TADA, SATOSHI WATANABE, Dept. of Materials Engineering, School of Engineering, The Univ. of Tokyo, CREST, Japan Science and Technology Agency — Four-probe measurements are powerful tools to investigate electric properties of materials precisely. Recently, the minimum probe spacing has reached to the order of 10 nm using nanotube probe tips [1]. However, it is not clear if the procedure used in macroscopic measurements can eliminate the effects of contact resistance even in such microscopic measurements. Keeping this in mind, we have developed a multi-probe transport simulator on the basis of Green’s function method combined with the density-functional tight-binding method [2]. So far, we have succeeded in self-consistent calculations at the limit of zero bias voltage for four-probe models consist of more than 1000 atoms, such as an infinite graphite ribbon with two or four semi-infinite nanotube tips. The calculation results indicate that the effects of the contact are not fully eliminated by the usual procedure.


1:39PM J20.00013 Quantum Blockades and Loop Currents in Graphene with Topological Defects, YAN-YANG ZHANG, JIANG-PING HU, B.A. BERNEVIG, XIANGRONG WANG, XIN-CHENG XIE, WU-MING LIU — We investigate the effect of topological defects on the transport properties of a narrow ballistic ribbon of graphene with zigzag edges. Our results show that the longitudinal conductance vanishes at several discrete Fermi energies where the system develops loop orbital electric currents with certain chirality. The chirality depends on the direction of the applied bias voltage and the sign of the local curvature created by the topological defects. This novel quantum blockade phenomenon provides a new way to generate a magnetic moment by an external electric field, which can prove useful in carbon electronics.

1:51PM J20.00014 Orbital Order in (LaMnO₃)ₘ(SrMnO₃)ₙ Superlattice, CHUNGWEI LIN, Physics Department, Columbia University, CLAUDE EDERER, School of Physics, Trinity College, ANDREW MILLIS, Physics Department, Columbia University — A realistic model for (LaMnO₃)ₘ(SrMnO₃)ₙ is constructed and solved by the semiclassical approximation. The model includes electron-electron, electron-lattice, and lattice-lattice interactions. Technically, we generalize the semiclassical approximation to the multi-orbital system and include the cooperative Jahn-Teller effect in the impurity problem. Within this framework, we present the orbital order in the superlattice.

This work is supported under DOE Grant No.ER-46169.

2:03PM J20.00015 Direct measurement of core-level relaxation dynamics on a surface adsorbate system, JING YIN, LUIS MIAJA-AVILA, GUIDO SAAHTOFF, CHAN LA-O-VORAKIAT, MARGARET MURNANE, HENRY KAPTEYN, JILA, University of Colorado, STEFAN MATHIAS, MARTIN AESCHLIMANN, University of Kaiserslautern, Germany, MICHAEL BAUER, Christian-Albrechts-Universität zu Kiel, Germany — Electronic coupling between an adsorbate and the surface on which it resides is fundamental to the understanding of many surface interactions. However, the interaction of highly-excited adsorbate states is an area that has been explored only indirectly to-date. In this work, we present the first direct time-resolved observations of the lifetime of core-excited states of an atom adsorbed onto a surface. By implementing laser-assisted Auger decay on an adsorbate/surface system, we directly measure the lifetime of the 4d⁻¹ core level of Xenon on Pt(111) to be 7.1 ± 1.1 fs. This result opens up time domain measurements of highly-excited state dynamics in systems where, because of complex interactions, energy-resolved measurements provide incomplete information.

Tuesday, March 11, 2008 11:15AM - 2:03PM —
Session J21 DCP: Focus Session: Clusters, Cluster Assemblies, Nanoscale Materials IV —
Convention Center 213

11:15AM J21.00001 Quantum Mechanics and Electrodynamics Studies of the Optical Properties of Metal Clusters/Nanoparticles, GEORGE SCHATZ, Northwestern University — This talk will describe the use of electrodynamics and quantum mechanics methods to describe the optical properties of silver and gold nanoparticles and other nanostructures. This work has been done in collaboration with several experimental colleagues, including Chad Mirkin, Rick Van Duyne and Teri Odom. Our recent work has focused on the optical properties of metal nanoparticles that are coated with molecules that are detected either through their influence on plasmon resonance excitation, or via surface enhanced Raman spectroscopy (SERS). Electrodynamics calculations using either the DDA or FDTD methods provide a quantitative tool for characterizing far field properties, and at a more primitive level estimates of SERS intensities. Quantum mechanics, as developed using time dependent density functional theory, is restricted to small metal clusters, but the same methods of far field spectroscopy and SERS can still be studied.

11:51AM J21.00002 Low Temperature Static Dipole Polarizability of Free Sodium Clusters with from 2 to 250 atoms, ANTHONY LIANG, JOHN BOWLAN, GaTech, XIAO- SHAN XU, SHUANG-YE YIN, WALT A. DE HEER, GaTech — The electric dipole polarizabilities of all sodium clusters Naₙ were measured from the atom up to n =250 using the molecular beam deflection method. Clusters were formed in cryogenic laser vaporization source operating at a temperature of 20 K. This complete sequence of high-resolution polarizabilities measurements greatly enhances previous experiments. Electronic shell effects are observed as well as several features that are not readily understood in the shell model. The asymptotic limit of the measurements appears not to converge to the bulk sodium polarizability value. The data are compared with theoretical predictions.

12:03PM J21.00003 Novel Properties of Diamondoid Molecules, WILLIAM CLAY, ZHI LIU, WANLI YANG COLLABORATION, ZHI-XUN SHEN COLLABORATION, NICK MELOSH COLLABORATION, JEREMY DAHL COLLABORATION, ROBERT CARLSON COLLABORATION — The recent isolation of a number of diamond-like hydrocarbons molecules (diamondoids) has sparked renewed interest in these unusual molecular systems. Several unique properties of these molecules are investigated. Diamondoid monolayers have been found to profoundly alter the electron emission tails of metal substrates in recent photoemission experiments, producing a sharp, nearly monochromatic peak. It is postulated that the cause of this effect is negative electron affinity combined with a strong electron-phonon interaction. New data and simulation results are presented to support this theory. Additionally, photoluminescence spectra for a number of diamondoid crystals are presented, taken with a 229 nm laser. To our knowledge, this is the first observation of UV photoluminescence in a saturated hydrocarbon molecule. Possible explanations for this phenomenon are discussed.
12:15PM J21.00004 Room temperature stability of mass selected Ag clusters on C_{60} functionalized surfaces. STEFANIE DUFFE, LUKAS PATRYARCHA, TORSTEN RICHTER, BENEDIKT SIEBEN, HEINZ HÖVEL, Technische Universität Dortmund, Experimentelle Physik I, Germany, CHUNRONG YIN, BERND VON ISSENDORFF, Universität Freiburg, Fakultät fuer Physik, Germany, MICHAEL MOSELER, Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg, Germany — Mass selected clusters from Ag^{−1}_{n=1} to Ag^{−3}_{n=5} were soft landed on HOPG and Au(111) functionalized with 1 and 2 monolayers (ML) of C_{60} molecules [1]. Depositions at 165 K gave extremely narrow cluster height distributions in STM images measured at 77 K. Using C_{60}/HOPG or 2 ML C_{60}/Au(111) the cluster heights are stable for more than 12h at room temperature (RT). For 1 ML C_{60}/Au(111) the cluster height decreases and finally all clusters disappear at RT. Molecular dynamics simulations reveal a process by which the clusters decay by atom through 1 ML C_{60}/Au(111) at RT. A sharp maximum at 1.7 nm cluster height forms during the cluster decay, indicating that there exists some metastable ‘supported magic number’.


1Work supported by the Deutsche Forschungsgemeinschaft (SPP 1153)

12:27PM J21.00005 Modification on the melting of aluminum nanoclusters by a copper atom: heat capacities of CuAl^{−n}_{n=1} nanoalloys, BAOPENG CAO, COLLEEN M. NEAL, ANNE M. STARACE, MARTIN F. JARROLD, Department of Chemistry, Indiana University, 800 E Kirkwood Ave., Bloomington, IN 47405 — The melting of alloy clusters is currently of great interest and emerging as an important research area. In this talk, we report the synthesis and melting transition of CuAl^{−n}_{n=1} nanoalloy clusters (n = 49 – 62). Heat capacities and melting behaviors have been determined for CuAl^{−n}_{n=1} nanoalloy clusters using a novel collision induced dissociation method and are compared with those of pure aluminum cluster Al^{n+m}_{n=1}. All these nanoalloys present a first order melting transition at temperatures well below the melting temperature of the bulk aluminum and the eutectic temperature of their bulk alloys. No eutectic characteristic is detected for these nanoalloy clusters. Upon substitution of Al with a single copper atom, the melting of pure aluminum clusters has been altered considerably. Size and charge effects of the doping atom on the melting of host nanoclusters are discussed.

1We thank the NSF for financial support.

12:39PM J21.00006 Forces between Functionalized Silica Nanoparticles, J. MATTHEW D. LANE, AHMED E. ISMAIL, MICHAEL CHANDROSS, GARY S. GREST, Sandia National Labs — Polymer-coated nanoparticles have a wide variety of applications, including drug delivery, adhesives, coatings, and magnetics. Although, the complexity of these nanoparticles precludes atomistic simulations of large numbers of nanoparticles in solution, it is possible to study the interaction between pairs of nanoparticles in an explicit solvent using molecular dynamics. From these simulations, we can compute the potential of mean force (PMF) between nanoparticles, which can be used in coarse-grained simulations at larger length and time scales. In particular, we present results for PMFs between polymer-grafted silica nanoparticles as a function of chain length, core size, and approach velocity. We report results for explicit-atom models of poly(ethylene oxide)-coated nanoparticles in water and alkylsilsane-coated nanoparticles in decane.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

12:51PM J21.00007 Photo-fragmentation of the closo-carboranes, JING LIU, DANQIN FENG, P.A. DOWBEN, Dept. of Physics and Astronomy, University of Nebraska-Lincoln, A.P. HITCHCOCK, Dept. of Chemistry, McMaster University, Canada, A.L.D. KILCOYNE, T. TYLISZCZAK, Advanced Light Source, Lawrence-Berkeley Laboratory, J.D. BOZEK, Stanford Synchrotron Radiation Laboratory, E. RÜHL, Institut für Physikalische Chemie, Freie Universität Berlin, Germany — Single and multi-atomic excitation and fragment ion formation of three isomeric carborane cage compounds [closo-1,2-orthocarborane, closo-1,7-metacarborane, closo-1,12-paracarborane (C_{12}B_{10}H_{12})] following B 1s and C 1s excitation were studied by time of flight mass analysis. The energetic cycles were constructed to gain some insights into some decomposition processes. CH^{+} or BH^{+} fragment dominates the single ion fragmentation of the closo-carboranes. Double ion fragmentation yields and charge separation mass spectra of all three isomers are generally quite similar in that H^{+} and BH^{+}/CH^{2+}/CH^{+} ion pairs, BH^{+}/CH^{+} and Y^{+}_{11} ion pairs (where Y = (BH) or (CH)), Y^{+}_{3} and Y^{+}_{4} ion pairs (where Y = (BH) or (CH)) yields dominate. The H^{+} and BH^{+}/CH^{+} ion pairs dominate at the B 1s threshold for ortho- and metacarborane, while Y^{+}_{11} and Y^{+}_{11} ion pairs (where Y = (BH) or (CH)) dominate the multi-fragmentation ion yield of paracarborane at the B1s threshold.

1:03PM J21.00008 Coupled quantum dot / quantum shell systems: optical gain, ultrafast charge transport, and single particle blinking, PATANJALI KAMBHAMPATI, D.M. SAGAR, EVA DIAS, SAMUEL SEWALL, RYAN COONEY, McGill University, AMY GRIMES, DOUGLAS ENGLISH, University of Maryland — The CdSe/ZnS/CdSe core/barrier/shell nanostructure forms an electronically coupled quantum system that is a spherical analog to the quantum well superlattice. The core’s brightness is enhanced via light harvesting by the shell. This material offers an opportunity to study charge transport in spherical nanoscale materials. Here, we present new results on the femtosecond dynamics of radial charge transport in these materials. With a combination of excitonic state selectivity and femtosecond time resolution, we monitor the ultrafast relaxation dynamics of either the core or the shell, having optically excited either phase. The femtosecond experiments reveal strong optical gain as well as evidence of spatially separated bieexcitons, and coupling between phases. Finally, we present single dot data on the two-color blinking kinetics of these coupled quantum dot quantum shell systems.

1:15PM J21.00009 Sampling of stable and metastable cluster structures by a first-principles Monte Carlo approach, RALF GEHRKE, KARSTEN REUTER, Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin — Size-selected nano-scale atomic clusters are now systematically becoming accessible in experiment, but characterizing their ground-state and metastable isomer ensemble averages from first principles requires a global and local exploration of vast configuration spaces. We here explore a first-principles Monte Carlo scheme to efficiently sample the minima of the corresponding total energy landscapes. The energetics is obtained at the density-functional theory level, using an all-electron local orbital basis set.

1:27PM J21.00010 The Effects of pH and Acid Type on Porous Alumina Formation, ADAM FRIEDMAN, DERRICK BRITTAI, LATIKA MENON, Northeastern University Dept. of Physics — Porous aluminum oxide prepared by anodization has an enormous variety of uses in nanomanufacturing, as it can be used as scaffolding to grow nanowires and tubes of exacting size specifications. However, there is no complete physical model for its growth. Three models in particular have been suggested in the past. We experimentally study the stability of porous alumina formation and the effects of changing anodization voltage, acid pH, and acid type. Using this information, we show that the models err in their primary assumptions, we pinpoint the location of these errors, and we suggest a method to correct them.

1:39PM J21.00011 Probing the Coulomb Barrier Towards Ionic Fragmentation, SHAUN ARD, NASRIN MIRSALEH-KOHAN, ROBERT COMPTON, University of Tennessee — Quintessential to understanding the stability of multiply charged anions (MCAs) is the characterization of the so-called “Coulomb Barrier” (CB) toward the loss of an excess electron and/or dissociation into charged fragments. The CB arises due to the superposition of the long-range Coulomb repulsion of the excess electron (or anion), and the short-range attractive polarization binding energy of the anion (or fragment). The CB adds to the stability of MCAs, often rendering thermodynamically unstable species to be metastable toward autodetachment or dissociation. The magnitude and shape of the CB is expected to depend heavily on the decay pathway. Whereas dissociation into charged fragments is often the lowest energy pathway for many MCAs, the vast majority of previous research has focused on electron loss. In this work, collision-induced dissociation (CID) is employed to study fragmentation of disulfonic diamions of increasing “length”. Energy threshold for the production of SO4_2^- plus its conjugate anion are used to estimate the magnitude of the Coulomb barrier to dissociation. These measured thresholds are compared with ab initio calculations of the dissociation energy. The relationship between these magnitudes and the distance between the excess charges will then be discussed.

1:51PM J21.00012 Vibrational modes in metal core-shell nanoparticles, A.S. KIRAKOSYAN, T.V. SHAH-BAZYAN, Jackson State University — We study the spectrum of lowest vibrational modes of bimetallic nanoparticles in dielectric surrounding. For solid spherical particles, the mode’s period and decay time are determined by the ratio of particle radius to longitudinal sound velocities in metal and outside medium, respectively. In contrast, in bimetallic nanoparticles, the dependence of both period and damping time on aspect ratio is highly non-monotonic. In particular, for Au/Ag core-shell nanoparticles, in a wide range of aspect ratios, the fundamental mode period is lower than in both Au and Ag solid particles of the same overall size, while the damping time exhibits a minimum at aspect ratios around 0.5. The unique acoustical signature of complex nanostructures allows unambiguous determination of their composition from ultrafast pump-probe and Raman spectroscopy measurements.

Tuesday, March 11, 2008 11:15AM - 1:39PM –
Session J22 DMP DPOLY: Organic Electronics, Photonics and Magnetics: Theory Morial Convention Center 214

11:15AM J22.00001 Dependence of Mobility on Density of Gap States in Organics by GAMEaS - Gate Modulated Activation Energy Spectroscopy, WOO-YOUNG SO, DAVID LANG, Columbia University, ARTHUR RAMIREZ, Alcatel-Lucent — We develop a spectroscopic method for determining the density of states (DOS) in the energy gap - Gate Modulated Activation Energy Spectroscopy (GAMEaS). We also report the relationship of these gap states to the mobility of organic field-effect-transistors (FETs). We find that the field-effect mobility is parameterized by two factors: (1) the free-carrier mobility and (2) the ratio of the free carrier density to the total carrier density induced by the gate bias. We show that the highest mobility FETs have shallow exponential band tails of localized states with characteristic slope of 1/kT at 300K. Most remarkably, state-of-the-art crystalline FETs fabricated from rubrene, pentacene, and tetracene all have a very high free-carrier mobility, up to 200cm2/Vsec at 300K, with the somewhat lower effective mobilities dominated by localized gap states. This strongly suggests that further improvements in device performance could be possible with enhanced material quality.

11:27AM J22.00002 Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study, DENIS ANDRIENKO, VALENTINA MARCON, KURT KREMER, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, JAMES KIRKPATRICK, JENNY NELSON, Department of Physics, Imperial College London, Prince Consort Road, London SW7 2BW, United Kingdom — Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Using atomistic molecular dynamics (MD) simulations we study columnar discotic phases formed by various polyaromatic hydrocarbons. Combining Kinetic Monte Carlo and MD trajectories a correlation between the material morphology and charge mobility is then established. We are able to reproduce the trends and magnitudes of mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique.

11:39AM J22.00003 Optical spectra and exchange-correlation effects in molecular crystals, NA SAI, University of Texas at Austin, MURilo L. TIAgO, Oak Ridge National Laboratory, JAMES R. CHELIKOWSKY, University of Texas at Austin, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — We report first-principles GW-Bethe Salpeter Equation and Quantum Monte Carlo calculations of the optical and electronic properties of molecular and crystalline rubrene (C20H16). We predict the formation of intermolecular, charge-transfer spin-singlet excitons with energies in close agreement with the observed yellow-green photoluminescence in rubrene microcrystals. In contrast, spin-triplet excitons are localized and intramolecular with a predicted phosphorescence at the red end of the optical spectrum. We find that the exchange energy plays a fundamental role in raising the energy of intramolecular spin-singlet excitons above the intermolecular ones. Exciton binding energies are predicted to be around 0.5 eV (spin singlet) to 1 eV (spin triplet). The calculated electronic gap is 2.8 eV. The theoretical absorption spectrum agrees very well with recent ellipsometry data.
Recently, a strategy was developed to perform continuous optimization of molecular properties, the linear combination of atomic potentials (LCAP) approach. This approach finds optimal structures among 10^4 molecular candidates with strong structural similarity, the TB-LCAP approach may provide an effective means of identifying structures with optimal properties.

1:15PM J22.00006 Inverse Molecular Design in a Tight-Binding Framework
DEQUAN XIAO, WEITAO YANG, Department of Chemistry, Duke University, Durham, NC 27708, DAVID BERATAN, Department of Chemistry and Department of Biochemistry, Duke University, Durham, NC 27708 — We consider the trapping of a moving electron by a polar impurity in an uncompensated organic semiconductor when the multipole moment of the impurity is coupled to an intramolecular vibration, a dynamical generalization of the Vannikov-Novikov dipole trap model. Due to the slow power-law dependence of the multipolar interaction, the vibrational coordinate shifts adiabatically with the approach of the charge carrier. The fast molecular motion can be decoupled from the electron’s translational motion to first approximation by transforming to the polaron basis, leading to a polaron binding energy which serves to enhance the propensity for the moving charge to be captured. For an isolated impurity, however, the transformed Hamiltonian contains a repulsive ponderomotive term not described in conventional polaron theory. The repulsion can outweigh the attractive force at long range, presenting a barrier to trap formation. [1] S. V. Novikov and A. V. Vannikov, Chem. Phys. 169 (1993) 21-33.

1:27PM J22.00007 Ab initio Evaluation of the Charge-Transfer Integrals and Band Structures of Phenanthroline-based Molecular Crystals
H. LI, J.-L. BREDAS, Georgia Institute of Technology, C. LENNARTZ, BASF Aktiengesellschaft, Germany — Ab initio calculations are carried out to study the charge-transport properties of phenanthroline-based molecular crystals, BCP and Bphen. The charge-transfer integrals in the two crystalline structures and in a quasi-1D chain model for BCP are evaluated based on: (i) a tight-binding approximation for dimers; (ii) the band structures of the periodic systems. In these compounds, the LUMO/LUMO+1 energetics of the isolated molecules are very close, which results in the LUMO and LUMO+1 orbitals both having significant contributions to the LUMO level in the dimer. In this case, the usual definition based on the electronic coupling between the two LUMO orbitals from each molecule cannot be applied to describe the charge-transfer characteristics in the dimer. A new definition of “effective transfer integrals” based on “mixed states” was proposed (H. Li, J.L. Bredas, and C. Lennartz, J. Chem. Phys. 126 (2007) 164704) to address this problem. Within the tight-binding approximation, the “effective transfer integrals” for both hole and electron transfers are found to be in very good agreement with the valence and conduction band dispersions obtained from plane-wave DFT calculations. We acknowledge many stimulating discussions with Vaclav C. Cojocaru and Demetrio da Silva Filho.

1This work has been supported by BASF, the Office of Naval Research under Award CHE-0443564, and the National Science Foundation under Award DMR-0120967.

1:39PM J22.00008 ABSTRACT WITHDRAWN

1:51PM J22.00009 Electron-phonon coupling in naphthalene crystal
ROEL SÁNCHEZ-CARRERA, PAVEL PARAMONOY, Department of Physics, University of Akron, Akron, Ohio 44325-4001, VEACESLAV COROPCEANU, JEAN-LUC BREDAS, School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400 — We investigate the electron-phonon couplings in naphthalene crystal. The electron-phonon couplings were evaluated by means of numerical differentiation; in this approach, the crystal geometry is distorted along normal modes and transfer integrals for several selected molecular pairs are then computed at each distorted geometry. We find that the DFT and force field results for phonon frequencies and electron-phonon couplings compare very well. Interestingly, several phonon modes are calculated to display significant quadratic electron-phonon coupling. In addition, we have also performed electronic band-structure calculations and derived the effective masses for both electrons and holes.

1:03PM J22.00010 Solid state effects on the photophysics of π-conjugated polymer thin films
ALOK SHUKLA, Indian Institute of Technology Bombay, ZHENHONG WANG, SUMIT MAZUMDAR, University of Arizona — The photophysics of thin films of π-conjugated polymers (PCPs) are remarkably different from that of dilute solutions. The difference is generally ascribed to interchain interactions and disorder in films. Microscopic understanding of the consequences of interchain interactions has remained incomplete in spite of intensive investigations. We present a theory of the complete energy spectrum of interacting PCP chains that leads to correct qualitative, and perhaps even semiquantitative description of the photophysics of PCP films. Within our theory of photoexcitations occurs to exciters that occur both below and above the optical excitation. Emission, as well as ultrafast photoinduced absorption (PA) in films are from the lower excimer. The lowest energy PA at 0.35 - 0.4 eV corresponds to the allowed transition from the lower eximer to the lowest polaron-pair. We explain why the energies of the PA at ~ 1.0 eV and higher are the same in films and solutions, even though the origins of these PAs are different. Finally, we give consistent explanations of the peculiarities associated with emission in films, including delayed emission, its quenching by electric field and the reappearance of the delayed emission upon removal of the field.

1Supported by NSF-DMR-0705163

1:15PM J22.00011 ABSTRACT WITHDRAWN
report on comprehensive quantitative analyses of x-ray diffuse scattering studies of nanoscale inhomogeneities in the optimally doped YBCO superconductor.

ISLAM, Argonne National Laboratory (ANL), SUNIL SINHA, UCSD, SIMON MOSS, University of Houston, JONATHAN LANG, ULRICH WELP, ANL — We doped yttrium barium copper oxide superconductor $^{1}$ simple Arrhenius and stretched-exponential relaxations and can be best described by the model of anomalous diffusion on the appropriate hypersphere. We time-dependence of the spin- spin correlation function in this material by means of Neutron Spin Echo (NSE) spectroscopy. Our high-precision NSE data exclude found that they can be understood in the framework of an effective anisotropic 3D random field Ising model. Here we report on the measurement of the neutron scattering, we have investigated the nano-scale structure of short-range charge and spin ordering in a half-doped cobablite La$_{1.5}$Sr$_{0.5}$CoO$_{4}$, and stripe indicated critical behavior expected from a two dimensional magnetically ordered state, whereas the site associated with the charge stripe showed three axis) character. Muon relaxation confirmed this to be consistent with a single magnetically ordered spin stripe phase. The muon site associated with the spin at 70 K to 57.4 $^{1}$ indicating a glassy transition to the ordered phase, in agreement with the susceptibility. Neutron diffraction determined a second magnetic transition that is

$^{1}$This work was supported in part by ONR. R. Allen was supported by the ASEE research fellowship program.

Tuesday, March 11, 2008 11:15AM - 2:15PM — Session J23 DMP GMAG: Focus Session: Cuprates and Nickelates Morial Convention Center 215

11:15AM J23.00001 Unidirectional charge modulations in underdoped cuprates observed with STM $^{1}$, J. C. DAVIS, Cornell University — No abstract available.

11:51AM J23.00002 Phase Separation and Magnetism in High Tc Superconductors $^{1}$, SAMUEL EMERY, BARRETT WELLS, HASHINI MOHOTTALA, JOSEPH BUDNICK, WILLIAM HINES, Univ. of Connecticut, LINDA UDBY, KIM LEMFANN, NEILS HESSEL ANDERSEN, Risoe National Laboratory, CHRISTOF NIEDERMAYER, NIERS CHRISTENSEN, ETH Zurich and Paul Scherrer Inst., JEFFREY LYNN, NIST, FANGCHENG CHOU, National Taiwan Univ. — Previous work by our group has determined that the low temperature phase diagram of super- oxygenated, La$_2$CuO$_4$ consists of only a few line phases that are either superconducting (SC) or magnetic. Samples with doping levels between the stable phases will segregate into separate domains; this raises the question as to the nature of the interaction between SC and magnetic domains. We have begun a neutron scattering study of the magnetic behavior of two such crystals. The oxidation states vary such that in one sample we have a phase separation between a low Tc (30K) SC phase and a striped magnetic phase, while the other features a high Tc (40K) SC phase and striped magnetic phase. Elastic neutron scattering reveals little field dependence of the magnetic peaks in the former, while in the latter we see an enhancement of the magnetic intensity. We also are deriving a method for separating contributions to the inelastic magnetic scattering by the SC and magnetic phases.

$^{1}$Work supported by the DOE grant DE-FG02-00ER45801

12:03PM J23.00003 Spin order and dynamics in a low doped nickelate $^{1}$, ANDREI SAVICI, Johns Hopkins University, IGOR ZALIZNYAK, GENDA GU, Brookhaven national Laboratory, VASILE GARLEA, Oak Ridge national laboratory — Due to their similarities with high-Tc cuprates, doped 214 layered nickelates attract significant interest. We have recently performed elastic and inelastic neutron scattering experiments studying the low-Sr-doped material La$_{1.55}$Sr$_{0.45}$NiO$_4$. This sample has nominal hole concentration similar to that in optimally doped cuprate superconductors. We observe static spin and charge ordering patterns and dynamic spin correlations, which we will compare to those arising from one dimensional physics expected in the stripe picture.

12:15PM J23.00004 Detection of the Spin Reorientation and Glassy Dynamics in La$_{1.55}$Sr$_{0.45}$NiO$_4$ $^{1}$, SEAN GIBLIN, ISIS, Rutherford Appleton Lab, PAUL FREEMAN, ILL, France, DHARMALINGHAM PRABHAKARAN, ANDREW BOOTHROYD, University of Oxford, UK — the magnetism of charge stripe ordered La$_{1.55}$Sr$_{0.45}$NiO$_4$ was studied by the combined techniques of neutron diffraction, spin relaxation and mass susceptibility. Magnetic ordering was observed at a lower temperature by muon relaxation than neutron diffraction, indicating a glazy transition to the ordered phase, in agreement with the susceptibility. Neutron diffraction determined a second magnetic transition that is observed by all techniques, to be a spin reorientation. On cooling below $T_{f} = 12$ K the spins re-orientate from lying 33.7 $^{1}$ away from the stripe direction at 70 K to 57.4 $^{1}$ away at 10 K. The magnetic order was observed by neutron diffraction to be of both anisotropic 3D and 2D (without any correlation on the $c$ axis) character. Muon relaxation confirmed this to be consistent with a single magnetically ordered spin stripe phase. The muon site associated with the spin stripe indicated critical behavior expected from a two dimensional magnetically ordered state, whereas the site associated with the charge stripe showed three dimensional critical behavior indicating spin frustration at the charge stripe.

12:27PM J23.00005 Anomalous diffusion on a hypersphere and time structure of two-point spin correlations in short-range-ordered doped oxides, $^{1}$, IGOR ZALIZNYAK, Brookhaven National Laboratory, GEORG EHLERS, Oak Ridge National Laboratory, GENDA GU, Brookhaven National Laboratory — Recently, much attention was paid to exploring charge and spin-ordered phases in strongly correlated transition metal oxides, such as superconducting cuprates and related nickelates, manganites and cobaltites. Using elastic neutron scattering, we have investigated the nano-scale structure of short-range charge and spin ordering in a half-doped cobaltite La$_{1.55}$Sr$_{0.45}$CoO$_4$, and found that they can be understood in the framework of an effective anisotropic 3D random field Ising model. Here we report on the measurement of the time-dependence of the spin correlation function in this material by means of Neutron Spin Echo (NSE) spectroscopy. Our high-precision NSE data exclude simple Arrhenius and stretched-exponential relaxations and can be best described by the model of anomalous diffusion on the appropriate hypersphere. We argue that such time dependence is generic for short-range-ordered spin systems.

$^{1}$Supported under DoE Contract DE-AC02-98CH10886 and NSF grant DMR-0454672.

12:39PM J23.00006 Transverse displacement modulation of the 1D metallic chains in optimally doped yttrium barium copper oxide superconductor $^{1}$, XUERONG LIU, University of California San Diego (UCSD), ZAHIRUL ISLAM, Argonne National Laboratory (ANL), SUNIL SINGHA, UCSD, SIMON MOSS, University of Houston, JONATHAN LANG, ULIRCH WELP, ANL — We report on comprehensive quantitative analyses of x-ray diffuse scattering studies of the 1D metallic chains in optimally doped YBCO superconductor $^{1}$. In addition to previously studied $q_{y} = \left(1, 0, 0\right)$ superstructure due to oxygen vacancy ordered ORTHO-IV phase and Huang diffuse scattering due to coherent long-range strain, we present a clear x-ray scattering observation of a transverse displacement modulation of the 1D CuO$_2$ metallic chains. This modulation co-exists within the well-formed ORTHO-IV patches and persists at temperatures well below $T_{c}$. Interestingly, the periodicity of this modulation is close to that of $\frac{1}{2} a_{x}$ according to electronic band calculations. The significance of these modulation and their role in the formation of the electronic inhomogeneities on a nano-meter length scales will be discussed.

$^{1}$Use of the Advanced Photon Source is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.
12:51 PM J23.00007 Investigation of a Model for the Magnetic Properties of RuSr$_2$GdCu$_2$O$_8$ based on the Temperature Dependence of Mössbauer Spectra$^1$. D. COFFEY, M. DEMARCO, Dept. of Physics, Buffalo State College, NY 14222, B. DABROWSKI, S. KOLENSIK, M. MAXWELL, Dept. of Physics, Northern Illinois University, DeKalb, IL 60115, S. TOORONGIAN, M. HAKA, Nuclear Medicine Department, State University of New York, NY 14260 — Mössbauer spectra were measured from 4.2K to 145K on a $^{197}$Ru enriched sample of RuSr$_2$GdCu$_2$O$_8$ which magnetically orders at 138K and has a full transition to superconductivity at 8.7K with an onset at ∼13K. The superconducting transition has no effect on the spectrum which is determined by the hyperfine magnetic field. At low temperatures there is a rapid decrease of this hyperfine magnetic field with increasing temperature indicating a gapless magnon spectrum. We use a local moment model which includes coupling between nearest neighbor in-plane Ru moments and between the Ru moments and Gd moments to calculate the magnon spectrum and use this to estimate the strength of the exchange interactions based on the hyperfine field temperature dependence. The coupling strength is ∼250K for Ru-Ru coupling and ∼15K for Ru-Gd coupling. We discuss the possible microscopic origin of these coupling strengths.

$^1$The work was supported by the USDOE(DE-FG02-03ER46064) at BSC and by the NSF(DMR-0302617) at NIU.

1:03 PM J23.00008 Layer Dependence of Charge Distribution and Electronic Structure of HgBa$_2$Ca$_2$Cu$_2$O$_{12+}$ $^2$, WEI-GUO YIN, DMITRI VOLJA, WEI KU, Brookhaven National Laboratory, WARREN PICKETT, University of California,Davis, DEEPA KASINATHAN, Max-Planck Institute for Chemical Physics of Solids — Recent experimental observation of layer-dependent properties of the five-layer superconducting cuprate HgBa$_2$Ca$_2$Cu$_2$O$_{12+}$ has inspired extensive interest. In general, multi-layer cuprates are of great interest because the influence of the apical oxygen $p_z$ states, the main source of the material dependence of cuprate structural and electronic properties [1], could be significantly layer-dependent. In this talk, the layer dependence of the charge distribution and electronic structure of HgBa$_2$Ca$_2$Cu$_2$O$_{12}$ will be investigated via the recently developed many-body Wannier-state method [1]. Possible implications on modulation of local pairing gaps, hole mobility, “super-repulsion” [1], and electron-phonon interaction among these distinct Cu$_2$O$_2$ layers will be discussed, in connection with the intriguing experimental findings of coexisting superconducting and antiferromagnetic orders as well as strong interlayer charge inhomogeneity. Work partially supported by DOE-CMSN. [1] W.-G. Yin and W. Ku, cond-mat/0702469.

1:15 PM J23.00009 Electron doping of cuprates via interfaces with manganites $^3$, ELLIO DAGOTTO, Department of Physics and Astronomy, The University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, SEIJI YUNOKI, ADRIANA MOREO, Department of Physics and Astronomy, The University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory, SRIVENKATESWARA KANCHARLA, Materials Science and Technology Division, Oak Ridge National Laboratory, ATSUHI FUJIMORI, Department of Physics, University of Tokyo — The possible electron doping of some overdoped high-$T_c$ cuprates via the transfer of charge from undoped manganites (or other oxides) using heterostructure geometries is discussed theoretically [1]. An analysis of photoemission and differential voltage experiments locate the Fermi level of some manganites above the bottom of the upper Hubbard band of some cuprate parent compounds. The addition of electrons to antiferromagnetic Cu oxides may lead to a superconducting state at the interface with minimal quenched disorder. Model calculations support this view. [1] S. Yunoki et al., Phys. Rev. B 76, 064532 (2007) and references therein.

$^3$Work supported by DOE & DOE-CMSN.

1:27 PM J23.00010 Tuning Hole Mobility, Distribution and Repulsion in High-$T_c$ Cuprates via Apical Atoms$^1$, WEI KU, CMPMSD, Brookhaven National Lab; Physics Department, State University of New York, Stony Brook, WEI-GUO YIN, CMPMSD, Brookhaven National Lab — Using a newly developed first-principles Wannier-states approach that takes into account large on-site Coulomb repulsion, we derive the low-energy effective one-band interacting Hamiltonians for several prototypical cuprate superconductors. The material dependence is found to originate primarily from the different energy of the apical oxygen $p_z$ state. Specifically, the general properties of the low-energy hole state, namely the Zhang-Rice singlet, are significantly modified, via additional intra-sublattice hoppings, near-neighbor “super-repulsion,” and other microscopic many-body processes. Possible implications on modulation of local pairing gaps, charge distribution, hole mobility, electron-phonon interaction, and multilayer effects will be discussed.

$^1$Work supported by DOE & DOE-CMSN.

1:39 PM J23.00011 Mid-IR band in cuprates : A consequence of strong electron correlations, SHILADITYA CHAKRABORTY, University of Illinois at Urbana - Champaign, DIMITRIOS GALANAKIS, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Optical conductivity data in lightly doped cuprates show an anomalous peak - like feature in the mid-IR regime not naturally expected of doped Mott insulators. Investigating this phenomenon in the light of strong electron correlations, we employ Cluster Dynamical Mean Field Theory (CDMFT) on a four site square plaquette to compute the optical conductivity in the 2-d Hubbard model as a function of hole doping and temperature. The computed optical conductivity shows a peak in the mid-IR regime, consistent with experimental data. Using Non - Crossing Approximation (NCA) as our impurity solver for CDMFT, we have identified the plaquette eigenstates that give rise to the mid-IR feature. The relevant eigenstate has 4 electrons on a plaquette with zero total spin and spatial properties consistent with $d_{x^2-y^2}$ symmetry.

1:51 PM J23.00012 Fluctuation corrections to the conductivity and the Hall conductivity near a spin–density–wave quantum critical point$^1$, JIE LIN, ANDREW MILLIS, Department of Physics, Columbia University — On the mean field level, the presence of the spin density wave order gives rise to distinct features in the transport properties of the electron–doped cuprates, which agree qualitatively with experimental data. Here, we determine how fluctuations modify the mean field behavior of the conductivity and the Hall conductivity, with particular attention to the vicinity of the quantum critical point. We developed a theory that respects the spin rotation symmetry. We determine the electron–spin fluctuation vertex and thus the transport and spectral properties of the electrons. Our formulation leads to a correctly gauge-invariant description with particular attention to the vicinity of the quantum critical point. We determine the general properties of the low-energy hole state, namely the Zhang-Rice singlet, are significantly modified, via additional intra-sublattice hoppings, near-neighbor “super-repulsion,” and other microscopic many-body processes. Possible implications on modulation of local pairing gaps, charge distribution, hole mobility, electron-phonon interaction, and multilayer effects will be discussed.

$^1$Research supported by NSF-DMR-0705847

2:03 PM J23.00013 Inhomogeneous phases of itinerant antiferromagnets, LEONID ISAEV, GERARDO ORTIZ, Indiana University - Dep. of Physics, CRISTIAN D. BATISTA, Los Alamos National Lab — Although magnetic properties of high-Tc cuprates and heavy fermion compounds have received great attention, only little investigation was performed in the purely antiferromagnetic (AF) phases of these materials. For instance, the mechanism of suppression of the magnetic order was never addressed. In the present work we use a 3D repulsive Hubbard model in an external magnetic field with anisotropic hopping parameters to show that this suppression occurs through a sequence of inhomogeneous states, which are coexisting charge/spin density waves and can be mapped onto the usual Larkin-Ovchinnikov states of type-II superconductors. At the mean-field level we compute the phase diagram of this model as a function of doping and lattice anisotropy. It is shown that morphology of the inhomogeneous phases is determined by the topology of the Fermi surface, which is controlled by the anisotropy (Lifshitz transitions). Insight into the properties of collective modes, such as damping, is gained by computing the magnetic response function in the random phase approximation. Our results are directly applicable to the striped phase of the nickels and may be useful for understanding the interplay between AF and superconducting orders in the underdoped phase of high-Tc and heavy fermion materials.
Tuesday, March 11, 2008 11:15AM - 2:15PM —
Session J24 DMP: Focus Session: Optical Properties of Nanostructures IV: Quantum Dots
Morial Convention Center 216

11:15AM J24.00001 Assessment of carrier multiplication in semiconductor nanocrystals by transient photoluminescence spectroscopy, GAUTHAM NAIR, SCOTT GEYER, MOUNGI BAWENDI, Massachusetts Institute of Technology — The enhancement of carrier multiplication (CM) is an important aim that could increase solar cell performance and widen the range of materials suitable for future solar technologies. Pump-probe measurements have shown evidence of strongly enhanced CM in lead chalcogenide, InAs, and CdSe nanocrystals (NCs). However, the nature of the enhancement mechanism is not well understood. We have carried out an experimental assessment of CM yields in semiconductor NCs by carefully studying exciton and biexciton signatures in transient photoluminescence decays. In the case of CdSe NCs, though the technique is particularly sensitive due to the biexciton’s relatively fast radiative rate, we have found no evidence for CM up to photon energies as high as 3.1 Eg. This result is strongly in disagreement with previous reports on CM in CdSe NCs. The implications of our findings on the efficiency and material dependence of CM are discussed within a general physical framework.

11:27AM J24.00002 The shape and symmetry dependence of excitonic radiative decay in CdSe nanocrystals, QINGZHONG ZHAO, ALBERTO FRANCESCHETTI, PETER A. GRAF, WESLEY B. JONES, KWINSEON KIM, National Renewable Energy Laboratory, LIN-WANG WANG, Lawrence Berkeley National Laboratory — For the last decade, the exciton recombination dynamics of nanocrystal quantum dots (NQDs) through radiative decay have been extensively studied by experimental and theoretical methods, because some NQDs, like CdSe and CdS/ZnS, show near unity quantum yield. Using atomistic, semiempirical pseudopotential calculations, we investigate the radiative decay of band-edge excitons in CdSe nanocrystals with perfect and imperfect shapes. While the lifetimes of bright excitons are in the nanosecond range and not sensitive to size and shape, we find that the radiative lifetimes of the ground state dark excitons are highly dependent on the surface shape and symmetry. The introduction of one [100] or [111] facet can drastically reduce the dark exciton lifetime from milliseconds to microseconds, and such faceting is observed by STEM. This provides an alternative to the explanation by spin-flip assisted or surface-assisted recombination mechanisms of the observed microsecond dark exciton lifetime. Our results highlight the importance of QD surface shape and broken symmetry in exciton dynamics.

11:39AM J24.00003 Peculiar many-body effects revealed in the spectroscopy of highly charged quantum dots, M. EDIGER, Heriot Watt University, GABRIEL BESTER, National Renewable Energy Laboratory, A. BADOLATO, P. PETROFF, University of Santa Barbara, K. KARRAI, Ludwig-Maximilians-Universität, A. ZUNGER, National Renewable Energy Lab, R. WARBURTON, Heriot Watt University, NREL COLLABORATION, HERIOT WATT COLLABORATION, LMU COLLABORATION, UCSB COLLABORATION — We have discovered new consequences of Coulomb interactions in self-assembled quantum dots by interpreting experimental spectra with results of atomistic pseudopotential calculations. The Coulomb effects are evident in the photon emission process and we can tune them in situ by controlling the quantum dot charge in the range from −6e to +6e. We find two regimes in the same dot: J ≤ ΔE for electron charging yet J ≃ ΔE for hole charging. We discover a breakdown of the Aufbau principle for holes; clear proof of non-perturbative hole-hole interactions; promotion-demotion processes in the final state of the emission process; and pronounced configuration hybridizations in the initial state. The level of charge control and the energy scales result in Coulomb effects with no obvious analogues in atomic physics.

11:51AM J24.00004 Anomalous Polarization Behavior of a Zeeman Doublet in CdSe Nanocrystal Quantum Dots, H. HTOON, Chemistry Division, Los Alamos National Laboratory, M. FURIS, S. A. CROOKER, National High Magnetic Field Laboratory, Los Alamos, AL, L. EFROS, Center for Computational Material Science, Naval Research Laboratory, S. JEONG, V. I. KLIMOV, Chemistry Division, Los Alamos National Laboratory — It is well known that a Zeeman doublet observed in emission spectra of a degenerate quantum state in the case of detection along an applied magnetic field (B field) is characterized by left and right circular polarizations. However, our single nanocrystal quantum dot (NQD) studies conducted in B-fields up to 5 T indicate that the Zeeman doublet of some of the CdSe NQDs exhibits a completely different polarization behavior. Specifically, we observe that the lower-energy state of the doublet becomes increasingly circularly polarized with increasing B field, while the higher-energy state shows a zero degree of circular polarization (i.e. remains linearly polarized). We explain this anomalous polarization behavior in terms of mixing between the Zeeman split levels derived from the low- and high-energy bright exciton states. This mixing relies on strong long-range electron-hole exchange interactions that are unique to ultrasmall nanocrystals.

12:03PM J24.00005 Influence of the electronic structure and the multi-exciton spectral density on the multiple exciton generation in semiconductor nanocrystals, CHRISTOPHE DELERUE, IEMN-ISEN, Lille, France, GUY ALLAN, IEMN-ISEN — Several experimental works have reported that a single high-energy photon could generate multiple excitons in semiconductor nanocrystals and several theories are proposed to explain these results. We calculate the electronic structure of InAs, Si and PbSe nanocrystals and we investigate two models of the multiple exciton generation (MEG). We show that the impact ionization process is efficient at high energy, with lifetimes as small as 10 fs. We present simulations of the MEG showing that, in PbSe and Si nanocrystals, the impact ionization alone cannot explain the observed efficiencies, even without relaxation by electron-phonon scattering. We calculate the spectral densities of multi-exciton states and we evaluate the possibility of direct photo-generation of multi-excitons. We confirm the importance of the multi-exciton spectral densities because of their rapid variation over several orders of magnitude. The high MEG efficiencies in PbSe and Si nanocrystals imply a very efficient relaxation in multi-exciton states characterized by a negligible density.

12:15PM J24.00006 State-resolved optical pumping and single exciton gain in CdSe quantum dots, RYAN COONEY, PATANJALI KAMBHAMPATI, SAMUEL SEWALL, D.M. SAGAR, McGill University — Optical gain in semiconductor quantum dots has been under intense investigation. Optical gain has been difficult to produce unless special geometries were employed such as thin films of CdSe quantum dots, or more recently, type II CdS/ZnS core/shell structures. The prototypical CdSe quantum dots in dispersion typically show small gain even at extremely high carrier concentrations. The key problem is induced absorptions due to multi-exciton interactions which result in losses that cancel the expected gain. Our recent state-selective approach can be used to prepare initial excitonic states, which has yielded much insight on exciton relaxation dynamics. This approach was used here to generate some of the largest gains ever measured, at the lowest thresholds, for all sizes of CdSe quantum dots in dispersion. These results show that gain in quantum dots is general, if the system is driven correctly.
12:27PM J24.00007 Optical conditional gates in laterally coupled quantum dots: the role of electron-hole exchange interaction. SOPHIA ECKDOMOU, THOMAS REINECKE, Naval Research Lab — We propose a fast, optically induced two-qubit C-PHASE gate in laterally coupled quantum dots. We use a model potential with two asymmetric local minima to account for the difference in size and composition of the two dots. By making use of the excited bound states of the total potential, which extend over both dots and which gives rise to an effective coupling between the two resident electron spins, we avoid the need for an external bias, such as that typically used in vertically coupled dots. The electron-hole exchange interaction is shown to play an important role in our proposal. By lowering the symmetry of the eigenstates, it allows for a simple design of a fast (about 50 ps) C-PHASE gate. The dissipative dynamics of the excited states have been taken into account in our numerical simulation of the fidelity. The calculated fidelity depends on the values of the decay rates. Our proposal is consistent with the single qubit operations we proposed [Phys. Rev. Lett. 99, 217401 (2007)], and the combination of the two allows for universal quantum gates.

12:39PM J24.00008 Fine Structure of Charged Excitons and Multiexcitons in Self-Assembled InGaAs/GaAs Quantum Dots. VLADAN MLINAR, JUN-WEI LUO, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, Colorado 80401 — As a quantum-dot is loaded with Ne electrons and Nh holes, complex charged excitons and multiexcitons are formed. Their fingerprint is the splitting of each exciton line into a set of multiplets separated by “fine structure” splitting, whose calculation [1] poses a serious test to many-body theories. Previously, such fine-structure splittings were calculated and measured for charged excitons with (Ne,Nh) of (2,1), (1,2), (3,1), and (1,3), demonstrating good agreement with experiment. Here, we extend the calculation to both charged and neutral multiexcitons with (Ne,Nh) of (2,2), (3,2), (2,3), (3,3), (4,3), (3,4), and (4,4). The energy splittings, oscillator strength, and polarizations of the optical emission are obtained from many body pseudopotential calculations. We present here predictions for the optical emission from negatively and positively charged biexcitons which reveal fine structure splittings in the order of 100 micro-eV, within the experimental accuracy of single dot micro photoluminescence. We will discuss the evolution of the patterns of multiplet lines, their spacings, and regularities vs. the number of particles (Ne,Nh). [1] M. Ediger, G. Bester, et al., Phys. Rev. Lett 98, 36808 (2007).

12:51PM J24.00009 Absorption spectroscopy of quantum dot molecules. DANNY KIM, Naval Research Laboratory, M.F. DOTY, University of Delaware, M. BASKHANSKY, M. SCHEINBER, A.S. BRACKER, D. GAMMON, Naval Research Laboratory — The energy levels of a vertically-coupled self-assembled InAs/GaAs quantum dot pair are probed using differential transmission spectroscopy. This technique offers very fine spectral resolution (< 0.1 µeV) allowing us to resolve the linewidths and fine structure for the various energy levels found in the rich spectrum of coupled quantum dots. For example, we observe increased broadening of the neutral exciton as it approaches the anticrossing point, as a result of a non-zero tunneling term well away from resonance. Excitons particular to coupled dots — i.e. a positive trion/biexciton, where the additional hole is on the spectator dot — exhibit polarization and power-dependent behavior that is in marked contrast to their single dot counterparts. Finally, the occupation of these exciton states are manipulated by using a second laser that is resonant on a related energy level. These experiments are a crucial step in using these molecules for coherent nonlinear optical processes.

1:03PM J24.00010 Förster optical signatures in quantum dot molecule photoluminescence. JUAN E. ROLON, SERGIO E. ULLOA, Ohio University — We formulate a realistic model that predicts the optical signatures of the Förster resonant energy transfer processes (FRET) in InAs/GaAs self-assembled quantum dot molecules (QDMs) in presence of laser illumination and electric fields. We study the time evolution of a multie excitonic Hamiltonian and construct a map of its dressed spectrum, resulting in effective coupling of the different states under laser illumination. In addition to interdot hole- and electron-tunneling, FRET is found to be an important quantum coupling mechanism in QDMs. We find FRET optical signatures to be highly dependent on structural parameters and severely constrained by the narrow spectral overlap between excitonic transitions in the donor-acceptor pair. However, detailed analysis of the orbital character of the localized hole reveals that it is possible to obtain strong spectral overlap between the first excited single exciton level in the donor dot and the lowest energy single exciton level in the acceptor dot. Remarkably, although FRET occurs via a single pair of exciton levels, its effects are evident throughout the calculated dressed spectrum. We observe a redistribution of spectral weights of direct and Stark shifted exciton lines, and a set of anticrossings among exciton states not directly coupled by FRET. Our results suggest experimental schemes to quantify FRET in photoluminescence experiments.

1:15PM J24.00011 Excited-state absorption and quantum confined Stark effect in embedded silicon and germanium nanocrystals. CEYHUN BULUTAY, Bilkent University — Realistic-sized Si and Ge nanocrystals (NCs) embedded in wide band-gap matrices are studied theoretically using an atomistic pseudopotential Hamiltonian. Based on this electronic structure, first the interband absorption is studied which shows the importance of surface polarization effects that significantly reduce the absorption when included. This reduction is found to increase with decreasing NC size or with increasing permittivity mismatch between the NC core and the host matrix. The intraconduction and interband absorption coefficients are also obtained in the wavelengths range from far-infrared to visible region. Next, we introduce the Stark effect which leads to an effective coupling between the two resident electron spins, we avoid the need for an external bias, such as that typically used in vertically coupled dots. Molecular resonances between energy levels of the two QDs are measured purely optical as sequences of anti-crossing patterns in the electric field dependent PL spectrum. These sequences provide in situ characterization of the level structure. We anticipate that such measurements will precede more sophisticated quantum control demonstrations, allow precise reverse engineering and boost detailed theoretical modeling of QD structures. This work is supported by NSA/ARO.

1Supported by TUBITAK with the Project No. 106T048

1:27PM J24.00012 Level Anti-Crossing Spectroscopy - Optically Mapping the Electronic Structure of Coupled Quantum Dots1, M. SCHEINBER, M. YAKES, A. S. BRACKER, I. V. PONOMAREV, M. F. DOTY2, C. S. HELLBERG, L. J. WHITMAN, T. L. REINECKE, D. GAMMON, Naval Research Laboratory — We introduce an all optical anti-crossing spectroscopy (LACS) with which the ground and the excited state energy levels of quantum dot (QDs) can be measured for a hole(electron) by itself and in the presence of other charges. Analogies are drawn to the atomistic shell-model and connections are made in an average way to structural STM measurements. An applied bias provides an electric field between two InAs/GaAs QDs which “tilts” the energy levels of both QDs relative to each other. Molecular resonances between energy levels of the two QDs are measured purely optical as sequences of anti-crossing patterns in the electric field dependent PL spectrum. These sequences provide in situ characterization of the level structure. We anticipate that such measurements will precede more sophisticated quantum control demonstrations, allow precise reverse engineering and boost detailed theoretical modeling of QD structures. This work is supported by NSA/ARO.

1submitted for publication

2Now at University of Delaware
Although the model predictions are consistent with classical cooperativity signatures, stable intermediates appear, in violation of the two-state assumption. The extent to which hybridization in solution conforms to two-state thermodynamics is also analyzed. Monte Carlo simulations with parallel tempering are routinely carried out to quantify and to interpret genomic information. At a surface, molecular interactions are amplified by the two-dimensional nature of the immobilized layer which focuses the nucleic acid charge and concentration to levels not encountered in solution, and which impacts the hybridization behavior in unique ways. We find that, at low ionic strengths, an electrostatic balance between the concentration of immobilized oligonucleotide charge and solution ionic strength governs the onset of hybridization. As ionic strength increases, the importance of electrostatics diminishes and the hybridization behavior becomes more complex. Suppression of hybridization affinity constants relative to solution values, and their weakened dependence on the concentration of DNA counterions, indicate that the immobilized strands form complexes. Moreover, an unusual regime is observed in which the surface coverage of immobilized oligonucleotides does not significantly influence the hybridization behavior, despite physical closeness and hence compulsory interactions between sites. These results are interpreted and summarized in a diagram of hybridization regimes.

Tuesday, March 11, 2008 11:15AM - 2:15PM –
Session J25 DPOLY DBP: Focus Session: Biopolymers: Molecules, Solutions and Networks I
Morial Convention Center 217

11:15AM J25.00001 Conformation and Trapping of DNA at a Convergent Stagnation Point . JENNIFER KREFT, Department of Chemistry, University of Texas, Tyler, YENG-LONG CHEN, Institute of Physics, Academia Sinica, HSUEH-CHIA CHANG, Chemical and Biomedical Engineering, University of Notre Dame — We use a lattice-Boltzmann based Brownian dynamics simulation to investigate the elongation of DNA at a convergent stagnation point trapped by a uniform attractive potential. Surprisingly, we find that the coiled state is favored over the stretched state at high Peclet number, Pe. The final elongation is determined by conformation changes during transport to the stagnation point, rather than hydrodynamic stretching at that point. The trapping rate of the DNA is consistent with the classical mean-field convection-diffusion theory and scales as $Pe^{1/3}$. This scaling is insensitive to the attractive potential used.

11:27AM J25.00002 DNA Surface Hybridization Regimes . RASTISLAV LEVICKY, Polytechnic University, PING GONG, Columbia University — Surface hybridization reactions, in which sequence-specific recognition occurs between immobilized and solution nucleic acids, are routinely carried out to quantify and to interpret genomic information. At a surface, molecular interactions are amplified by the two-dimensional nature of the immobilized layer which focuses the nucleic acid charge and concentration to levels not encountered in solution, and which impacts the hybridization behavior in unique ways. We find that, at low ionic strengths, an electrostatic balance between the concentration of immobilized oligonucleotide charge and solution ionic strength governs the onset of hybridization. As ionic strength increases, the importance of electrostatics diminishes and the hybridization behavior becomes more complex. Suppression of hybridization affinity constants relative to solution values, and their weakened dependence on the concentration of DNA counterions, indicate that the immobilized strands form complexes. Moreover, an unusual regime is observed in which the surface coverage of immobilized oligonucleotides does not significantly influence the hybridization behavior, despite physical closeness and hence compulsory interactions between sites. These results are interpreted and summarized in a diagram of hybridization regimes.

11:39AM J25.00003 Hybridization Pathways and Mechanisms of Model DNA Oligonucleotides in Solution . JUAN ARAQUE, Rice University, ATHANASSIOS PANAGIOTOPoulos, Princeton University, MARC ROBERT, Rice University — We propose a coarse-grained lattice model of short DNA strands to investigate the microscopic pathways and mechanisms of oligonucleotides hybridization in solution. The extent to which hybridization in solution conforms to two-state thermodynamics is also analyzed. Monte Carlo simulations with parallel tempering are performed to estimate the equilibrium population of single- and double-stranded states and the associated free-energy landscapes. Sequence complexity is shown to largely dominate the nucleation and helix propagation pathways. The two-state nature of the transition is found to exhibit strong sequence dependence. Although the model predictions are consistent with classical cooperativity signatures, stable intermediates appear, in violation of the two-state assumption.

1:39PM J24.00013 Charged Quantum Dots in High Quality Micropillar Cavities . MATTHEW RAKHER, Physics Dept., University of California Santa Barbara, NICK STOLTZ, LARRY COLDREN, PIERRE PETROFF, Materials Dept., University of California Santa Barbara, DIRK BOUWMEESTER, Physics Dept., University of California Santa Barbara — We report on nanodevices that for the first time allow for charge tuning of single InAs quantum dots located near the field maximum of high quality micropillar cavities. Through the innovation of a novel trench style cavity design, we are able to embed doped layers for electrical gating within a microcavity and obtain Q values greater than 50,000. Using these devices, we demonstrate record high single photon count rates with a capture efficiency of 38% and a Purcell effect up to 8. We also show high frequency polarization modulation of single photons enabled by Stark shift tuning a charged quantum dot between two polarization modes of a slightly elliptical micropillar with frequencies up to 100 kHz. Furthermore, we demonstrate a charge tunable quantum dot coupled to a micropillar cavity mode, which is an important step in quantum communication protocols involving trapped single electrons or holes. This type of device enables a quick, non-destructive measurement of the spin state of the trapped charge.

2:03PM J24.00015 Control of sp-d exchange interactions in pseudo-type II Mn:ZnSe/CdSe core-shell nanocrystal quantum dots . DAVID BUSSIDAN, MING YIN, LANL, SCOTT CROOKER, NHMFL, LANL, VICTOR KLIMOV, LANL — Dilute magnetic semiconductors (DMSs) have been the focus of considerable research due to their potential usability in spin-based electronic devices. Unpaired electrons of dopant atoms, such as Mn$^{2+}$, can couple strongly to electrons of the semiconductor (sp-d exchange interaction), which should allow for the manipulation of the spin degree of freedom using traditional microelectronic circuitry. We have developed a novel approach for manipulating sp-d interactions between the dopant and the semiconductor wherein Mn ions are incorporated into cores of ZnSe/CdSe core-shell semiconductor nanocrystal quantum dots (QDQs). These NCs represent quasi-type II hetero-structures that allow one to tune both the band edge transition energy and dopant-carrier wavefunction overlap by changing the size of the core and/or shell thickness. We will report our recent results from a set of doped heterostructures for which we demonstrate tunability of both the magnitude and the sign of the sp-d exchange interaction energy as a function of hetero-NQD geometry.

1:51PM J24.00014 Photoluminescence spectra of thin films containing CdSe/ZnS quantum dots irradiated by 532-nm laser radiation and gamma-rays . SURESH SHARMA, JAY MURPHREE, TONMOY CHAKRABORTY, AJANI ROSS, CECIL SHIVE, University of Texas at Arlington — We have investigated temporal behavior of the photoluminescence (PL) spectra of thin films containing CdSe/ZnS quantum dots irradiated by 532 nm laser radiation and gamma-rays. Under $\sim 100$ W/cm$^2$ laser radiation, the PL intensity ($I_{PL}$) increases with irradiation time up to about 500s and thereafter declines linearly. The wavelength of the PL emission ($\lambda_{peak}$) exhibits a blue-shift with exposure time. Upon simultaneous irradiation by 100 W/cm$^2$ 532-nm laser, as well as 0.57 and 1.06 MeV gamma-rays, the temporal behaviors of both $I_{PL}$ and $\lambda_{peak}$ are significantly different; $I_{PL}$ increases to a saturation level, and the magnitude of the blue-shift in $\lambda_{peak}$ is reduced. We also present data on the effects of the density of the quantum dots on the temporal behavior of the PL spectra, as well as additional data on samples synthesized with CdSe/ZnS quantum dots embedded in conducting polymer films. We discuss possible mechanisms underlying our observations.

Supported in part by a grant from Strategic Partnership of Research in Nanotechnology (SPRING) administered by Air Force Office of Scientific Research.
11:51 AM J25.00004 Structure and applications of a temperature responsive recombinant protein hydrogel based on silk- and elastin-like amino acid motifs, LAWRENCE DRUMMY, MELANIE TOMCZAK, Air Force Research Laboratory, JOSEPH MACAULIFFE, Genencor Inc., RICHARD VAIA, RAJESH NAIK, Air Force Research Laboratory — Proteins form the main components of many natural materials, and they can be designed to offer tailored functionality and material properties. Silk elastin-like proteins (SELPs) come from a family of repeat sequence protein polymers based on Bombyx mori silk and mammalian elastin that are recombiantly expressed in E. coli. SELP gels are formed by heating the protein solutions in order to induce physical crosslinking of the silk β-sheet regions, they contain approximately 80-90% water by weight and they can be used for encapsulation of enzymes or nanoparticles. For example, horseradish peroxidase demonstrates added resistance to drying and heat treatment on the gel morphology. During gel formation, small angle X-ray scattering shows intensity increases in two distinct regions of reciprocal space, one reversible with temperature and one irreversible. By fitting the scattering data to a unified power-law/Gunier model, morphological parameters are extracted. The thermally reversible intensity changes are attributed to a hydrophilic/hydrophobic transition in the elastin segments, while the irreversible intensity change is due to the crystalline regions formed by the silk blocks.

12:03 PM J25.00005 Fractal Nature of Semiflexible Networks in beta-Hairpin Peptide Hydrogels, ROHAN HULE, DARRIN POCHAN, Materials Science and Engineering, University of Delaware — De novo designed beta hairpin peptides with asymmetric beta strands, capable of self-assembly and hydrogel formation, were investigated. The stimuli responsive self-assembly occurs via a strand-interdigitation mechanism, resulting in physically crosslinked fibrillar networks. Fibrils with distinct nanostructures varying from non-twisted, twisted to laminated morphologies were rationally designed by modulating the peptide strand registry. The fractal dimension and correlation lengths of these networks, both, at the network as well as individual fibril length scales vary significantly with concentration and is directly related to the fibril morphology, as evidenced by SAXS and cryogenic TEM. In case of the laminated fibrils, an increase in the peptide concentration induces a change from surface to mass fractal behavior at high q due to the disruption of fibril lamination as a result of faster assembly kinetics from higher peptide concentration. Non-twisting peptide fibril morphologies exhibit an increase the network density with higher peptide concentration and, therefore, an increase in mass fractal dimension. Oscillatory rheology of hydrogels reveals enhanced moduli for laminating networks over non-twisting or twisting networks. These interdigitating peptides constitute a model system to study structure-property relations in other semiflexible networks.

12:15 PM J25.00006 A molecular model for toughening in double-network hydrogels, WEN-LI WU, VIJAY TIRUMALA, NIST, TAIKI TOMINAGA, Hokkaido University, SANGHUN LEE, PAUL BUTLER, ERIC LIN, NIST, JIAN PING, GONG, HIDEUMITSU FURUKAWA, Hokkaido University — A molecular mechanism is proposed for the toughness enhancement in double network (DN) hydrogels prepared from poly (2acrylamido, 2-methyl,1-propanesulfonicacid) (PAMPS) polyelectrolyte network and polyacrylamide (PAAm) linear polymer. It is an extension of the phenomenological model set forth recently by Gong et al. This mechanism takes into consideration all the observed changes in molecular structure of the constituents during the single neutron scattering (SANS) measurements, the composition dependence of the solution viscosity and the thermodynamic interaction parameters of PAMPS and PAAm molecules from our previous neutron scattering studies. More specifically, this proposed mechanism provides an explanation of the observed periodic compositional fluctuation in the micrometer range induced by large strain deformation.

12:27 PM J25.00007 De novo designed peptide and peptide-polymer conjugate for biomolecular materials, TING XU, University of California, Berkeley — Peptides, nature’s “own” building blocks, provide control of functional groups over nanometer distances with sub-Angstrom resolution and can be de novo designed to self-assemble into multidimensional molecular constructs that mimic natural proteins or perform functions not found in nature. Conjugating synthetic peptides to polymers, forming peptide-polymer conjugates, takes advantages of both the stability and processibility of synthetic polymers and the built-in peptide functions. Helical bundles, a ubiquitous folding motif, underpin many structural and catalytic functions of natural proteins. By attaching a polymer chain to a helical bundle-forming peptide, the polymer chain will mediate the interactions between the helical bundle and its external environment, enable the macroscopic self-assembly and, potentially, allow the helical bundle to function in non-biological environments. A new design of peptide-polymer conjugates will be presented where the polymer chain is covalently linked to the side chain of the peptide. Upon attaching poly(ethylene glycol) (PEG) to the exterior of the helix bundle, the peptide secondary structure and also the tertiary structure, i.e., coiled-coil helix bundle formation, are stabilized. More importantly, using a photoactive heme-binding 4-helix bundle peptide as an example, this new design preserves the built-in functionalities in the interior of the helix bundle.

1:03 PM J25.00008 Single polymer stretching in elastic turbulence of polymer solution, YONGGANG LIU, VICTOR STEINBERG, Department of Physics of Complex Systems, Weizmann Institute of Science — Coil-stretch transition of single T4 DNA molecule in an elastic turbulence is studied in a polymer solution with the same molecules. Two mechanisms of saturation of polymer stretching in elastic turbulence, the nonlinearity of polymer stretching and the back reaction of stretched polymer chains to the flow, are demonstrated based on experiments of single polymer dynamics at different polymer concentrations. The elastic stress calculated from single polymer stretching agrees with the PIV measurement of the flow properties, indicating that polymer stretching can be used as an elastic stress probe of the flow properties.

1:15 PM J25.00009 Shape and conformation of confined biopolymers,1, YA LIU, BULBUL CHAKRABORTY, Brandeis University — Biological macromolecules living in cells are confined on length scales comparable to their intrinsic persistence length. In these environments, the bending rigidity plays a decisive role in determining shape and conformations. We have used numerical simulations to investigate the statistical properties of a semiflexible polymer confined in a square box. Simulations exhibit a sharp transition when the bare persistence length becomes comparable to the box size. An order parameter is introduced to quantify and analyze the nature of this transition. The shape change is accompanied by a qualitative change in the effective persistence length, which starts differing significantly from the intrinsic persistence length. A mean-field model, including Gaussian fluctuations around the saddle point solution, provides a quantitative description of the evolution of the tangent-tangent correlation function with increasing confinement.

1:27 PM J25.00010 Raft Formation of Rod-like Polyelectrolytes1, DANIEL W. SINKOVITS, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — We investigate the formation of raft-like aggregates by charged rod-like polyelectrolytes, as reported from experiments employing F-actin as well as from theoretical analyses. Through extensive molecular-dynamics simulations of pairs of rods at different salt concentrations we construct free-energy landscapes, which in turn elucidate the most likely kinetic pathways to aggregation. Additional simulations of layers of rods at varying skew orientations and lateral spacings demonstrate to what extent the lessons learned from pair simulations apply to large aggregates.

1:39 PM J25.00011 Vapor-liquid coexistence of patchy attractive fluids: Wertheim theory study, HONGJUN LIU, SANAT KUMAR, Columbia University, GLENN EVANS, Oregon State University — Our system consists of spherical particles whose pair potential contains hard core repulsion, short-ranged square well attraction and several distributed attractive patches on its surface. The simplicity of the model makes it possible to compare simulations and theoretical predictions based on Wertheim’s thermodynamic perturbation theory (TPT). Wertheim’s TPT is in good agreement with simulation data. In the broader parameter ranges, we show the patchy hard sphere fluids obey a generalized law of corresponding states (GLCS) and GLCS seems to hold for all patchy square well fluids with four to six interaction sites.
1:51PM J25.00012 Strong Keratin-like Nanofibers Made of Globular Protein, YAEI DROR, VADIM MAKAROV, Technion, Mechanical Eng. Dep., ARIE ADNON, Technion, Biology Dep., EYAL ZUSSMAN, Technion, Mechanical Eng. Dep. — Protein fibers as elementary structural and functional elements in nature inspire the engineering of protein-based products for versatile bio-medical applications. We have recently used the electrospraying process to fabricate strong sub-micron fibers made solely of serum albumin (SA). This raises the challenges of turning a globular non-viscous protein solution into a polymer-like spinnable solution and producing keratin-like fibers enriched in inter S-S bridges. A stable spinning process was achieved by using SA solution in a rich trifluoroethanol-water mixture with \(\beta\)-mercaptoethanol. The breakage of the intra disulfide bridges, as identified by mass spectrometry, together with the denaturing alcohol, enabled a pronounced expansion of the protein. This in turn, affects the rheological properties of the solution. X-ray diffraction pattern of the fibers revealed equatorial orientation, indicating the alignment of structures along the fiber axis. The mechanical properties reached remarkable average values (Young’s modulus of 1.6GPa, and max stress of 36MPa) as compared to other fibrous protein nanofibers. These significant results are attributed to both the alignment and inter disulfide bonds (cross linking) that were formed by spontaneous post-spinning oxidation.

2:03PM J25.00013 Electrosprinning of Natural Polymers\(^1\), AIHUA HE, Institute of Chemistry, Chinese Academy of Sciences, SHANSHAN XU, HUARONG NIE, JUNXING LI, CHARLES C. HAN, STATE KEY LAB OF POLYMER PHYSICS AND CHEMISTRY, INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCES — Electrosprinning is an effective and simple method to fabricate polymer fibers in the range of nano scale. However, electrosprinning of natural polymers is a challenge. The key reason for this problem is that natural polymers have very different chain conformation and hydrodynamic responses in solution, especially in aqueous solution, when compared with synthesized polymers. The objective of our study is to find the key parameters in order to have a good control in the electrosprinning process. We studied the electrosprinnings of gelatin from its aqueous solution, of hyaluronic acid without airblowing, and of pure alginate. It was found that electrosprinning of those natural-polymer solutions could be successfully carried out when key parameters were properly adjusted, such as viscosity, elasticity (chain entanglement) and surface tension.

\(^1\)Supported by the NSFC.

Tuesday, March 11, 2008 11:15AM - 1:51PM –
Session J26 DCP: Focus Session: Quantum Control I Morial Convention Center 218

11:15AM J26.00001 Quantum Control of Femtochemistry in the Gas Phase, Liquid Phase and on Surfaces, GUSTAV GERBER, Univ. of Wurzburg, Institute of Physics — By using coherent control techniques we control the behavior of quantum systems on their natural time scale, by applying ultrashort coherent light fields in the wavelength range from the IR to the UV. These laser pulses can be variably shaped in space and time using a laser pulse shaper consisting of a liquid-crystal display \([1]\). Laser-optimized femtochemistry in the gas phase and liquid phase is one field in which this new technique is successfully employed. Automated optimization of branching ratios and total product yields of gas phase photodissociation reactions as well as chemically selective molecular excitation in the liquid phase is performed \([2]\)\([3]\). Structural changes of a molecule in the liquid phase have been controlled by laser-optimized photoisomerization of a cyanine dye molecule \([4]\) and of retinal in bacteriorhodopsin \([5]\). So far, optimal control techniques have been restricted to gas phase and condensed phase optimization experiments. Recently we have demonstrated femtosecond laser-assisted catalytic reactions on a Pd(100) single crystal surface. By applying a closed-loop optimal control scheme, we manipulate these reactions and selectively optimize the ratio of different bond-forming reaction channels, in contrast to previous quantum control experiments aiming at bond-cleavage. The results represent a first step towards selective photocatalysis of molecules.


11:51AM J26.00002 Quantum control spectroscopy with multipulses, MARCUS MOTZKUS, Philipps Universität Marburg — The manipulation of molecular vibrations by laser light has been always considered as a very promising means to control chemical reaction. The coherently controlled time-dependent superposition of vibrational states may represent motion along a reaction coordinate and therefore allows for a high degree of selectivity. Pulse shapes for manipulating vibrations can be predicted to be trains of pulses with temporal spacing between the sub-pulses equal to an integer of the vibrational phase. If the manipulation of molecular vibrations with pulse trains is expected to be one of the important mechanisms on the natural standing time of mode selective chemistry, it is necessary to understand its application limits. In this work, the interaction of pulse trains with matter is discussed under the light of time-resolved nonlinear experiments and density matrix simulations. Emphasis is given to the role of electronic coherence between excited and ground-state, to the excited state population relaxation time and to the electronic resonance. In particular the lifetime of the excited state poses a challenge for the coherent control with multipulses and, thus, for the mode filtering capability in the excited state. This is investigated by applying a shaped femtosecond excitation pulse to different molecules in solution and probing the response by transient absorption, nonlinear Raman and DFWM spectroscopy. Finally, the effect of the phase of sinusoidal modulation on the envelope of the multipulse sequence and its consequences on pump-probe spectroscopy is discussed, particularly near zero delay between pump and probe pulses.

12:27PM J26.00003 Strategies for optimal control in complex systems, ROLAND MITRIĆ, Department of Chemistry, Humboldt-University Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany — We present strategies for the optimal control of the ground and excited state dynamics in complex systems, based on the combination of the quantum chemical molecular dynamics ‘on the fly’ with the semiclassical Wigner distribution approach \([1]\). We first demonstrate our strategy for the optimal control of the ground state dynamics based on the MD ‘on the fly’ with explicit treatment of the interaction with the laser field which is optimized using a genetic algorithm \([2]\). This approach will be illustrated on two prototype systems representing rigid symmetrical molecules and floppy biomolecules with low frequency modes. Our results show that the ground state isomerization process can be selectively driven by ultrashort laser pulses with different shapes which are characteristic for the prototype systems. Furthermore, for the optimal pump-dump control involving ground and excited electronic states we have developed a new ‘field induced surface hopping’ method in which the nuclear dynamics is treated classically while the laser induced electronic transitions are treated fully quantum mechanically. We illustrate our approach on the optimal control of cis-trans isomerization in prototype Schiff base molecular switches. Our theoretical approach allows us to explore the controllability of dynamics in complex systems and to unravel the mechanisms underlying the control of molecular processes. Furthermore, the outlook for laser selective photochemistry of nanoparticles and nanoparticle-biomolecule hybrid systems will be given.

et al. state are evaluated. [1] S. D. Kraft
creation of molecules. We present ab-initio calculations of excited molecular states of LiCs including spin-orbit coupling and study the alignment and orientation
the state distribution of the produced ground state molecules. Precise knowledge of the molecular structure is required to find the most efficient route for the
and detected with a high-resolution time-of-flight mass spectrometer [1]. Here we present the active photoassociation of ultracold LiCs molecules and discuss
a double species magneto optical trap. After spontaneous decay into the electronic ground state, the molecules were ionized by one-color two-photon ionization
formation of ultracold molecules through photoassociation of ultracold atoms. We recently observed the spontaneous formation of ultracold LiCs molecules in
A. GROCHOLA, R. WESTER, M. WEIDEMÜLLER, Albert-Ludwigs-University Freiburg, Germany, M. AYMAR, O. DULIEU, Laboratoire Aime Cotton, Orsay,
2 interpret the sharp peaks as signatures of bound states of psinons and antipsinons, fractional excitations in a magnetic field. We compare these spectral features
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in a magnetic field in terms of fractional excitations. Restricting the Hilbert space to that spanned by the eigenstates of the Heisenberg chain [1], we calculate
, MASANORI KOHNO, Computational Materials Science Center, NIMS, LEON BALENTS, Department of Physics, UCSB,
, ALBRECHT LINDINGER, FU Berlin — Optimal control
of photo-induced molecular processes has attained considerable success in recent years. An important issue in this regard is the information coded in the
optimized laser pulse shape which supplies insight about the underlying processes. Small alkali systems are suitable since they exhibit bound states available
for resonant transitions with weak fields which aids the theoretical description and thus the interpretation. New control methods are presented to extract the
most relevant information from the optimized laser field. Moreover, novel pulse shaper schemes for simultaneous phase, amplitude, and polarization pulse
control were designed and applied to alkali dimers, even in a parametric encoding. The results demonstrate the perspectives of adding the polarization and
hence all properties of the light field in the pulse modulation. Currently, coherent control was applied to ultracold ensembles motivated by the perspective to
perform photoassociation and photostabilization of alkali systems. First results are received regarding optimized multi-photon excitation to molecular ions and
pump-probe experiments exposing signal oscillations. They provide indications for photoassociation and open the perspective for transitions to lower vibrational
levels in the electronic ground state, which would be a first step to an internally cold molecular Bose Einstein condensate.
1:27PM J26.00006 Direct frequency comb measurement and control of vibrational dynamics
in ultracold molecular samples . AVI PE’ER, JILA, University of Colorado, EVGENY SHAPIRO, MOSHE SHAPIRO, University of British Columbia, Vancouver, JUN YE, JILA, University of Colorado and NIST — We propose a new class of control schemes for robust transfer of population between quantum states via a wave packet that utilize trains of coherent pulses (optical frequency comb). Our approach draws from analogy to adiabatic passage techniques in three-level systems, but is more general. We show that breaking a slow adiabatic passage into a train of short, perturbative pulses, enables highly

cold and ultracold molecular samples.
1:39PM J26.00007 Formation of a gas of ultracold LiCs molecules , J. DEGLMAYR, J. LANGE, S.D. KRAFT, A. GROCHOLA, R. WESTER, M. WEIDEMÜLLER, Albert-Ludwigs-University Freiburg, Germany, M. AYMAR, O. DULIEU, Laboratoire Aime Cotton, Orsay, France — Ultracold molecules offer intriguing perspectives for the study of many-body effects in strongly interacting gases and the manipulation by external
fields. A promising approach to the creation of a large ensemble of ultracold polar molecules in the absolute translational and electronic ground state is the direct
formation of ultracold molecules through photoassociation of ultracold atoms. We recently observed the spontaneous formation of ultracold LiCs molecules in
a double species magneto optical trap. After spontaneous decay into the electronic ground state, the molecules were ionized by one-color two-photon ionization
and detected with a high-resolution time-of-flight mass spectrometer [1]. Here we present the active photoassociation of ultracold LiCs molecules and discuss
the state distribution of the produced ground state molecules. Precise knowledge of the molecular structure is required to find the most efficient route for the
creation of molecules. We present ab-initio calculations of excited molecular states of LiCs including spin-orbit coupling and study the alignment and orientation

Tuesday, March 11, 2008 11:15AM - 2:15PM —
Session J27 GMAG: Focus Session: Triangular Lattice Morial Convention Center 219

11:15AM J27.00001 Mean filed study of disordered spin-\(\frac{1}{2}\) antiferromagnetic systems , VLADIMIR DOBROSALJEVIC, SEN ZOUH, Florida State University, EDUARDO MIRANDA, Universidade Estadual de Campinas — We present a mean field theory picture of disordered spin-\(\frac{1}{2}\) antiferromagnetic system as a function of the degree of disorder, in connection to the insulating doped semiconductors. The system is a resonant valence bond (RVB) liquid state at zero disorder, and a possible RVB glass state when the disorder is finite but weak. For a highly disordered system, we show that the essential physics is the formation and decimation of strongly coupled bonds, and the thermodynamics shows an effective power-law singularity, in qualitative agreement with renormalization group result of Bhatt and Lee.

11:27AM J27.00002 Dynamical properties of spatially anisotropic frustrated Heisenberg models in a magnetic field , MASANORI KOHNO, Computational Materials Science Center, NIMS, LEON BALENTS, Department of Physics, UCSB, OLEG. A. STARYKH, Department of Physics, University of Utah — We investigate spectral features of spatially anisotropic spin-1/2 frustrated antiferromagnets in a magnetic field in terms of fractional excitations. Restricting the Hilbert space to that spanned by the eigenstates of the Heisenberg chain [1], we calculate dynamical structure factor \(S(k,\omega)\) in the two-dimensional momentum space. We obtain sharp peaks and broad continuum depending on the momentum. We interpret the sharp peaks as signatures of bound states of psinons and antipsinons, fractional excitations in a magnetic field. We compare these spectral features with available experimental results on CuS\(\text{CuCl}_4\) [2], and make detailed predictions on momentum- and field-dependence of peak structures and line shapes of \(S(k,\omega)\) for CuS\(\text{CuCl}_4\) in a magnetic field. [1] M. Kohno, O. A. Starykh, and L. Balents, Nature Phys. 3, 790 (2007). [2] R. Coldea, et al., Phys. Rev. Lett. 79, 151 (1997).

11:39AM J27.00003 Quantum Order by Disorder in Frustrated Diamond Spinel Antiferromagnets , JEAN-SEBASTIAN BERNIER, MICHAEL J. LAWLER, YONG BAEK KIM, University of Toronto — We study the effect of quantum fluctuations on the frustrated diamond lattice antiferromagnet where frustration arises from the presence of second neighbor interactions. Such an antiferromagnet describes the magnetic properties of spinel \(\text{AB}_2X_4\) where magnetic ions are located on A-sites. We compare the resulting phase diagram of the quantum model and that of its classical counterpart, and discuss the difference/similarity between the quantum and thermal order by disorder phenomena. Implications for experiments on \(\text{CoRh}_2\text{O}_4\), \(\text{Co}_2\text{O}_3\), and \(\text{Mn}_2\text{Sc}_2\text{O}_4\) will be discussed.
11:51 AM  J27.00004  Random Fields and the Partially Paramagnetic State of CsCoO$_{3.93}$Mg$_{0.17}$Br$_3$
, JOHN-PAUL CASTELLAN, Argonne National Lab., MSD, B.D. GAULIN, McMaster University, W.J.L. BUYERS, NPMR, NRC, Chalk River Laboratories — Partially paramagnetic Neel states are among the exotic magnet states known to exist in nature as a consequence of geometrical frustration. This unusual magnetic structure occurs in the stacked triangular lattice antiferromagnets such as CsCoBr$_3$ and CsCoCl$_3$. CsCoBr$_3$ displays at least 2 magnetic phase transitions. The first, $T_{n1} \approx 28 K$ where the system enters a 3-sublattice state in which one of the sublattices remains disordered and the second, $T_{n2} \approx 13 K$ where the remaining disordered sublattice orders[1]. Critical neutron scattering measurements were performed on the doped system CsCo$_{1-x}$Mg$_x$Br$_3$ with $x=0.17$. We will discuss the evolution of the observed two component scattering below $T_{n1}$ in terms of a Random Field Ising model in both zero applied magnetic field and an applied magnetic field of 2.6T along the c-axis. [1] M.Mao et al. Phys. Rev. B 66, 184432 (2002).

12:03PM  J27.00005  New ordered phases of the spin-1/2 triangular-lattice antiferromagnet Cs$_2$CuBr$_4$
, NATHANALE FORTUNE, Smith College, SCOTT HANNAHS, National High Magnetic Field Laboratory, YASUO YOSHIDA, YASU TAKANO, University of Florida, TOSHI O NO, HIDEKAZU TANAKA, Tokyo Institute of Technology — Quantum fluctuations and geometric frustration are theoretically expected to produce a gapped, collinear ‘up-down’ phase in spin-1/2 Heisenberg and XY antiferromagnets on a triangular lattice. Experimentally, this phase should manifest itself as a magnetization plateau at 1/3 of the saturation value. Despite being a fundamental theoretical property of such systems, this behavior has to date only been observed in one triangular lattice antiferromagnet: Cs$_2$CuBr$_4$. We have investigated the magnetic phase diagram of this compound by means of specific-heat, magnetocaloric-effect, and magnetic torque measurements in magnetic fields up to the saturation field of about 30 T, finding a cascade of new ordered phases adjacent to the up-up-down phase. The evolution of these phases as a function of the field orientation with respect to the crystallographic bc plane suggests that they arise from the competition between the scalar exchange interaction and the symmetry-breaking Dzyaloshinskii-Moriya interaction.

12:15PM  J27.00006  Dynamics of the Spin Liquid Phase of Cs$_2$CuCl$_4$
, OOKIE MA, MARC-ANDRE VACHON, VESNA F. MITROVIC, BRAD MARSTON, Brown University — The dynamics of a spin-liquid phase of an antiferromagnet on the anisotropic triangular lattice and in a magnetic field are studied with a combination of Gutzwiller-projected wavefunctions and mean-field theory. Candidate ground states that support fermionic gapless spinon excitations include four different U(1) spin liquids. The lattice and the states interpolate between limiting cases of 1D decoupled chains ($J'/J = 0$) and the isotropic 2D square lattice ($J'/J = \infty$). Parameters of the mean-field theory are chosen to minimize the ground state energy of the corresponding Gutzwiller-projected wavefunction. The spin-lattice relaxation rate $1/T_1$, calculated within the mean-field approximation, is compared to NMR measurements in the spin liquid phase of Cs$_2$CuCl$_4$[1].

12:27PM  J27.00007  Photoemission study of triangular lattices in NiGa$_2$S$_4$, FeGa$_2$S$_4$, and Fe$_2$Ga$_2$S$_5$
, KOU TAKUBO, Department of Physics, University of Tokyo, TAKASHI MIZOKAWA, Dept. of Complexity Science and Engineering, Univ. of Tokyo, YUSUKE NAMBU, KEISUKE ONUMA, HIROSHI TONOMURA, OSAMU SAKAI, SATORU NAKATSUJI, YOSHIHITERO MAENO, Dept. of Physics, Kyoto Univ. — The newly-discovered NiGa$_2$S$_4$ (Ni$^{2+}$, S=1) and FeGa$_2$S$_4$ (Fe$^{2+}$, S=2) form frozen spin-disordered states within the triangular lattice [1,2]. The spins of both compounds have no long range order even at lowest temperature. We have performed photoemission spectroscopy of NiGa$_2$S$_4$, FeGa$_2$S$_4$, and Fe$_2$Ga$_2$S$_5$. The photoemission results and subsequent model calculations indicate that the ground state of NiGa$_2$S$_4$ has the $d^1_L$ character (L is a 3 $\bar{3}$p hole) and that the strong S $3p$ hole character of the ground state provides the enhanced superexchange interaction between the third nearest neighbor sites. In contrast, the ground state of FeGa$_2$S$_4$ is dominated by the $d^6$ configuration and the superexchange interactions between the second and third neighbor sites are less important. [1] S. Nakatsuji, et al., Science 309, 1697 (2005). [2] S. Nakatsuji, et al., Phys. Rev. Lett. 99, 157203 (2007).

12:39PM  J27.00008  The origin of anomalous 3rd neighbor exchange in 2D triangular magnets (NiGaS$_4$ and others)
, IGOR MAZIN, Center for Computational Materials Science, Naval Research Laboratory — 2D magnetic materials with triangular lattices have been attracting much interest. Among them one finds the parent compound of an exotic superconductor, Na$_2$CoO$_2$:yH$_2$O, A-type antiferromagnets like NaNiO$_2$, in-plane antiferromagnetism (LiCrO$_2$), spin-liquid type materials (NiGa$_2$S$_4$, charge-order (AgNiO)$_2$. The main structural motif in all of them is the AB$_3$ plane, where A is a transition metal and B is oxygen or sulfur. Experiments and calculations inevitably find anomalously strong 3rd neighbor exchange coupling in all these triangular planes, despite different band fillings and different magnetic ground states. I will explain why this happens, why this effect is so universal, and why it can be understood entirely on a one-electron level. I will use as an example NiGa$_2$S$_4$, with a reference to Na$_2$CoO$_2$ as well.

12:51PM  J27.00009  Elementary excitations in the spin liquid phase of Cs$_2$CuCl$_4$ as revealed by $^{133}$Cs NMR spin-lattice relaxation rate measurements.
, MARC-ANDRE VACHON, GEORGIOS KOUTROULAKIS, OOKIE MA, BRAD MARSTON, VESNA F. MITROVIC, Brown University, ARNEIL P. REYES, PHILIP L. KUHNS, NHMF, RADU COLDEA, Bristol University, Z. TYLCZYSKNI, Adam Mickiewicz University — We present $^{133}$Cs NMR spin-lattice relaxation rate measurements in the spin liquid phase of Cs$_2$CuCl$_4$ as a function of temperature and external magnetic field. At fixed temperature, we found that the rate increases with increasing field, reaching a maximum at a phase boundary of the spin liquid phase. The results are compared with the calculated NMR rates in different proposed spin liquid states. The implications of the results on determining the fermionic or bosonic nature of the elementary excitations in the spin liquid phase will be discussed.

1:03PM  J27.00010  Spin-1/2 Heisenberg Antiferromagnet on the Spatially Anisotropic Kagome Lattice
, ANDREAS SCHNYDER, Kavli Institute for Theoretical Physics, University of California, California, BART STARKKH, Department of Physics, University of Utah, LEON BALENDS, Physics Department, University of California, Santa Barbara — We study the quasi-one-dimensional limit of the Spin-1/2 quantum antiferromagnet on the Kagome lattice, a model Hamiltonian that might be of relevance for the mineral volborthite [1,2]. The lattice is divided into antiferromagnetic spin-chains (exchange $J$) that are weakly coupled via intermediate "dangling" spins (exchange $J'$. Using bosonization, renormalization group methods, and current algebra techniques we determine the ground state as a function of $J/J'$. The case of a strictly one-dimensional Kagome stripe is also discussed.

1:15PM J27.00011 Magnetic Order and Spin Fluctuations in the Spin-1/2 Three-Dimensional Frustrated Magnet Clinatoacamite, Cu$_2$(OH)$_3$Cl. JOEL HELTON, KITTIWIT MATAN, Massachusetts Institute of Technology, JAE-HO CHUNG, NIST Center for Neutron Research, MATTHEW SHORES, BART BARTLETT, EMMY NYTKO, Massachusetts Institute of Technology, YING CHEN, QINGZHEN HUANG, JEFFREY LYNN, NIST Center for Neutron Research, DANIEL NOCERA, YOUNG LEE, Massachusetts Institute of Technology — We have performed thermodynamic and neutron scattering measurements on the $S=1/2$ three-dimensional antiferromagnet clinatoacamite, Cu$_2$(OH)$_3$Cl. The crystal lattice feature Cu$^{2+}$ ions arranged on a distorted kagomé lattice with weak magnetic coupling between adjacent planes. Long range magnetic order with a weak ferromagnetic moment emerges at the Neél ordering temperature, $T_N = 6.2$ K. The value of $T_{CW}$ is roughly 30 times larger than $T_N$, demonstrating that the material is highly frustrated. Magnetic Bragg peaks are not observed above background for temperatures between 6.2 and 18 K, even though previous µSR measurements observed muon oscillations in this temperature range. We present a possible model of the magnetic transitions and analyze the inelastic spectrum of the ordered state, taking into account anisotropic terms in the spin Hamiltonian.

1:27PM J27.00012 Magnetic Properties of Yb$_2$Pt$_2$Pb with the Shastry-Sutherland Lattice. MOO SUNG KIM, Brookhaven National Laboratory, MARCUS BENNETT, University of Michigan, MEIGAN ARONSON, Brookhaven National Laboratory — We have synthesized single crystals of Yb$_2$Pt$_2$Pb, which crystallize in the tetragonal $P4_2$ $2$-Sn-type structure. Comparison of the crystal structure with that of other compounds reveals a structure dependent Yb valence state of Yb$^{2+}$ Tm$^3$ (T=transition metal; M=Cd, In, Sn, and Pb). The magnetic susceptibility $\chi$ of Yb$_2$Pt$_2$Pb is highly anisotropic. The $\chi_{[100]}$ for $B|[110]$ is 30 times larger than $\chi_{[001]}$ for $B|[001]$ at the lowest temperatures. A broad maximum in $\chi_{[100]}$ is found around 3 K just above magnetic transition temperature 2.07 K. In agreement, the electrical resistivity shows a broad maximum around 5 K and the specific heat shows a long tail up to 8 K, due to the magnetic frustration originating from antiferromagnetic exchange interaction between Yb ions arranged in the network of the Shastry-Sutherland lattice.

1:39PM J27.00013 Dynamic Frustration in PrAu$_2$(Si$_{1-x}$Ge$_x$)$_2$. RAYMOND OSBORN, EUGENE GOREMYCHKIN, Argonne National Laboratory, J.B. RAINFORD, University of Southampton, UK, ROBIN MACALUSO, University of Northern Colorado, D.T. ADROJA, Rutherford Appleton Laboratory, UK, MAREK KOZA, Institut Laue Langevin, France — We have recently proposed that frustration is dynamically induced in PrAu$_2$(Si$_{1-x}$Ge$_x$)$_2$. It has been demonstrated that these compounds have a structure dependent Yb valence state of Yb$^{2+}$ Tm$^3$ ($T = $transition metal; $M= $Cd, In, Sn, and Pb). The magnetic susceptibility $\chi$ of PrAu$_2$(Si$_{1-x}$Ge$_x$)$_2$ is highly anisotropic. The $\chi_{[100]}$ for $B|[110]$ is 30 times larger than $\chi_{[001]}$ for $B|[001]$ at the lowest temperatures. A broad maximum in $\chi_{[100]}$ is found around 3 K just above magnetic transition temperature 2.07 K. In agreement, the electrical resistivity shows a broad maximum around 5 K and the specific heat shows a long tail up to 8 K, due to the magnetic frustration originating from antiferromagnetic exchange interaction between Yb ions arranged in the network of the Shastry-Sutherland lattice.

1:51PM J27.00014 KTi(SO$_4$)$_2$.H$_2$O - a possible candidate for a new spin-Pierles system. DEEPA KASINATHAN, MPI CPS - Dresden, Germany, GORAN NILSEN, HENRIK RONNOW, LQM-EPFL, Lausanne, Switzerland, STEFAN-LUDWIG DRECHSLER, IFW Dresden, Germany, HELGE ROSNER, MPI CPS, Dresden, Germany — Recently a large number of compounds belonging to the family of J$_{(OH)}$ reveals that this system is a quasi 1D spin 1/2 chain compound with both J$_1$-J$_2$ chain models with competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions have been discovered. In most cases, FM-J$_1$ and AFM-J$_2$ is observed, leading to helical order with no spin gap (for frustration ratio $\alpha$). Models with competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions have been discovered. In most cases, FM-J$_1$ and AFM-J$_2$ is observed, leading to helical order with no spin gap (for frustration ratio $\alpha$). Systems with both J$_1$ and J$_2$ being AFM causing a spin gap are rather rare. The thermodynamic data of the recently prepared KTi(SO$_4$)$_2$.H$_2$O reveal that this system is a quasi 1D spin 1/2 chain compound with both J$_1$ and J$_2$ being AFM, and a frustration ratio $\alpha \approx 0.29$. Here we report the results of electronic structure calculations within the LSDA+U method along with tight-binding models. Our calculations confirm that both J$_1$ and J$_2$ are AFM. In contrast to the experiments we obtain a larger $\alpha$, slightly depending on the choice of the Coulomb repulsion $U$. Therefore KTi(SO$_4$)$_2$.H$_2$O might be a new candidate for a spin-Pierles ground state. A brief comparison with other systems belonging to the class of frustrated chain materials is given with respect to their position in the general phase diagram of the 1D J$_1$ - J$_2$ model.

2:03PM J27.00015 Valence bond solid phases in the spin-1 XXZ model on the kagome lattice. SERGEI ISAKOV, EUTH Zurich, YONG BAEK KIM, University of Toronto — We study the spin-1 XXZ model on the kagome lattice using quantum Monte Carlo simulations. We find a rich phase diagram including two different valence bond solids and other quantum paramagnetic phases. We also characterize the nature of quantum phase transitions between these phases. These results are compared with various effective field theory approaches.

Tuesday, March 11, 2008 11:15AM - 2:15PM – Session J28 DMP FIAP: Focus Session: Thermoelectricity in Semiconductor Nanostructures Morial Convention Center 220

11:15AM J28.00001 Theory of enhancement of thermoelectric properties of materials with nanoinclusions. SERGEY FALEEV, FRANCOIS LEONARD, Sandia National Laboratories — Based on the idea of Schottky potential as an energy filter for the electrons, we developed a theory that explains the enhancement of the thermoelectric properties of semiconductor materials with metallic nanoinclusions. The Boltzmann transport equation with relaxation time approximation is used for description of both electron and phonon scattering. The theory has been applied to optimize the ZT factor for n-doped PbTe with metallic nanoinclusions. We found that the contribution of electron scattering to optimized ZT is important for high electron concentration ($n \times 10^3$ cm$^{-3}$), while at low concentrations ($n \times 10^2$ cm$^{-3}$) enhancement of the ZT factor is primarily due to decrease of the phonon thermal conductivity.

11:27AM J28.00002 Measurement of Cross-plane Thermoelectric Properties of Thin Film Structures with UHV Scanning Thermoelectric Microscopy. YONG LEE, ANASTASIOS MAVROFEALOS, MICHAEL PETTES, LI SHI, The University of Texas at Austin — Recently, various thin film structures have been under intense research in the hope for achieving increased thermoelectric figure of merit (ZT) compared to bulk materials. Accurate measurements of three quantities ($S$ : Seebeck coefficient, $\sigma$ : electrical conductivity, and $\kappa$:thermal conductivity) used to calculate ZT have been a challenge especially for thin film structures which may have very different values between in-plane and cross-plane directions due to the anisotropy. Here, we report our progress toward accurately measuring these thermoelectric properties of thin films along the cross-plane direction with a ultrahigh vacuum (UHV) scanning probe microscope. In particular, cross-plane Seebeck coefficient and electrical conductivity measurement of a thin film with a conductive AFM or STM probe will be discussed.
11:39 AM J28.00003 Micro- and nanomachined tools for measuring thermopower and in-plane thermal conductivity of thermoelectric thin films, AZURE AVERY, RUBINA SULTAN, GREG STIEHL, BARRY ZINK, University of Denver. — Many of the potential next-generation thermoelectric materials being studied are either thin films or nanostructures that are expected to have anisotropic properties. Techniques such as the 3ω method and picosecond thermoreflectance allow accurate measurements of k⊥ at temperatures relevant to thermoelectrics, but measuring k∥ is often difficult. In this talk we discuss our efforts to design and demonstrate accurate measurements of k∥ of thin films from 77 – 475 K using micro- and nanomachined thermal isolation platforms. Using thin-film structures to support the thin-film sample reduces background contributions, and careful control of the geometry keeps radiation errors small. We will discuss the optimization and micromachining of the measurement platforms and their application for studying the growth and characteristics of our first doped amorphous thin films. We will present our first tests of the devices on materials established thermal properties. Finally, we will discuss the use of these measurement platforms to determine k and ZT for doped amorphous silicon thin films.

11:51 AM J28.00004 Thermopower and Electrical Conductivity of PbSe Nanocrystal Thin Films, ROBERT WANG, JOSEPH FESER, University of California, Berkeley, JONG-SOO LEE, DMITRI AL TALAPIN, University of Chicago, RACHEL SEGALMAN, ARUN MAJUMDAR, University of California, Berkeley — Thin films assembled of solution-processed PbSe nanocrystals have a thermopower 2 – 3 times greater than bulk PbSe. In addition, the thermopower and electrical conductivity both exhibit a size-dependence on nanocrystal size. As the nanocrystal diameter changes from 4 to 9 nm, the thermopower and electrical conductivity change from 850 to 650 μV/K and 10−1 to 10−2 S/cm, respectively. If electrical conductivity can be improved, these materials represent a new class of inexpensive and scalable thermoelectric materials.

12:03PM J28.00005 ABSTRACT WITHDRAWN

12:15PM J28.00006 First Principles Studies of Phonon Dispersion and Lattice Thermal Conductivity of Silicon Nanowires, TRINH VO, TADASHI OGITSU, ERIC SCHWEGLER, LLNL, GIULIA GALLI, UC Davis — We present phonon dispersions of Si nanowires using ab initio and linear response theory. The effects of nanowire surface structures, growth directions, and quantum confinement on phonon dispersions and phonon confinement are also discussed. The thermal conductivity of Si nanowires using the obtained full dispersion curves are also evaluated, using Boltzmann Transport Equation. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.

12:27PM J28.00007 Enhanced Thermoelectric Performance in Rough Silicon Nanowires1, RENKUN CHEN, Dept. of Mech. Engr., UC Berkeley, ALLON I. HOCHBAUM, RAUL DIAZ DELGADO, WENJIE LIANG, ERIK C. GARNETT, Dept. of Chemistry, UC Berkeley, MARK NAJARIAN, Dept. of Materials Sci. & Engr., UC Berkeley, ARUN MAJUMDAR, Dept. of Mech. Engr., UC Berkeley, PEIDONG YANG, Dept. of Chemistry, UC Berkeley — Due to the disparity between electron (<10 nm) and phonon (~100 nm) mean free paths in silicon, nanostructured Si could effectively block phonon transport by boundary scattering while maintaining electron transport, thereby enhancing thermoelectric figure of merit, ZT. Here we report the wafer-scale electrochemical synthesis and thermoelectric characterization of rough Si nanowires with enhanced ZT, relative to the bulk material. Single nanowire measurements show that their electrical resistivity and Seebeck coefficient are similar to those of bulk Si with similar dopant concentration. Thin nanowires, however, exhibit a 100-fold reduction in thermal conductivity (k), yielding a large ZT = 0.6 at room temperature. Although bulk Si is a poor thermoelectric material, Si nanowire arrays show promise as high-performance, scalable thermoelectric materials.

The authors acknowledge the support of the office of BES, DOE. A.I.H., R.C. and R.D.D. wish to thank the NSF-IGERT, ITRI-Taiwan and Gen-Cat/Fulbright programs, respectively, for support.

12:39PM J28.00008 Enhanced thermoelectric properties in silicon nanowires, SLOBODAN MITROVIC, JEN-KAN YU, AKRAM BOUKAI, JAMIL TAHIR-KHELI, WILLIAM A. GODDARD III, JAMES R. HEATH, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125. — Recently, we demonstrated that silicon nanowires can be designed and fabricated to achieve an approximately 100-fold enhancement in thermoelectric efficiency compared to bulk silicon. Independent measurements of thermoelectric power, and thermal and electrical conductivities suggest that this improvement is due to phonon effects rather than quantum confinement. Here, we present the study of the scaling laws (i.e. nanowire length/width dependence) for the phonon dynamics and transport. We investigate the influence of the phonon drag, carrier mobility and doping on the thermoelectric properties, and the universality of these findings. This work is supported by the Office of Naval Research, the Defense Advanced Research Projects Agency.

12:51PM J28.00009 Atomic Modeling and Optimization of thermoelectric properties of SiGe nanowires1, M. MARIA CHAN, YING SHIRLEY MENG, TIM MUELLER, GERBRAND CEDER, Massachusetts Institute of Technology, JOHN REED, TRINH VO, ANDREW WILLIAMSON2, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California, Davis. — Nano-structured thermoelectric materials have been shown experimentally to have superior figure of merit compared to bulk materials. To understand the origin of this superiority, it is of interest to develop physically accurate methods to compute the thermoelectric transport coefficients of nanowires. In addition, computationally inexpensive parameterization of these physical models are needed in order for efficient sampling, e.g. in atomic configuration space, so as to design systems with optimal thermoelectric properties. We consider aspects of electron and phonon transport in SiGe nanowires. For electronic transport, we work in the diffusive regime with Boltzmann transport, combining ab initio density functional theory (DFT) calculations with a perturbative treatment of electronic scattering to obtain electronic relaxation times, conductivity and thermopower. The phonon contribution to thermal conductivity is obtained from classical equilibrium molecular dynamics simulations using the Green-Kubo formalism. Cluster expansion and effective potential techniques are used to parameterize the transport coefficients for efficient sampling and optimization.

Funded by DARPA PROM (Predicting Real Optimized Materials) Program

(1)Supported by AFOSR, DOE
1:15PM J28.00011 Thermoelectric Properties of Semiconducting Silicide Nanowires, SONG JIN, JEANNINE SCZECH, JEREMY HIGGINs, University of Wisconsin-Madison, FENG ZHOU, LI SHI, University of Texas-Austin — Semiconducting silicides are promising thermoelectric materials. In addition to their respectable thermoelectric figure-of-merit ($ZT$ up to 0.8), silicides have the advantages of low cost, excellent thermal stability and mechanical strength, and outstanding oxidation resistance, making them suitable for high temperature applications. We have developed general synthetic approaches to single crystal nanowires of silicides to investigate the enhancement of thermoelectric properties due to the reduced nanoscale dimension and to explore their applications in thermoelectrics. We will discuss the synthesis and structural characterization of nanowires of chromium disilicide ($\text{CrSi}_2$) prepared via a chemical vapor transport (CVT) method and chemical vapor deposition (CVD) of organometallic precursors to synthesize the Novotnyon Chimney ladder phase MnSi$_{1.75}$. The Seebeck coefficient, electrical conductivity, and thermal conductivity of individual CrSi$_2$ nanowires were characterized using a suspended microdevice and correlated with the structural information obtained by microscopy on the same nanowires. This combined Seebeck coefficient and electrical conductivity measurements also allow an effective approach to probing the Fermi level, carrier concentration and mobility in nanowires. We will also discuss our progress in using individual nanostructures combined well-defined structural characterization to conclusively investigate the complex thermoelectric behaviors of silicide materials.

1:27PM J28.00012 Tuning of Thermoelectric Transport in Individual Bismuth Nanowires, ARDEN MOORE, MICHAEL PETTES, ANASTASSIOS MAVROKEFALOS, LI SHI, University of Texas-Austin — Bismuth is a material of special interest for studying nanoscale transport behavior. Its extremely small effective mass and long electron mean free path suggest that quantum and classical confinement effects might be observed at realistic dimensions and higher temperatures than in other material systems. In addition, the predicted enhancement of the thermoelectric figure of merit $ZT$ due to confinement effects of these systems increases the desire to measure the transport properties of individual bismuth nanowires. However, efforts to measure the thermoelectric properties of bismuth nanowires have been hindered thus far by the presence of a highly stable surface oxide layer, making reliable ohmic contact to individual nanowires problematic. In this work, we present the synthesis and measurement methods used by our group to make electrical contact with individual nanowires in order to measure the thermal conductivity, thermopower, and electrical conductivity of individual bismuth nanowires of varying diameter. The obtained data is presented with comparison to bulk values and analysis of the transport behavior.

1:39PM J28.00013 Thermopower Measurements of Pure and Sn (Te) Doped Bismuth Nanowires$^1$, TITO HUBER, Howard University. Washington DC 20059, A. ADEYEYE, Howard University. Washington, DC 20059, A. NIkolaeVA, L. KONOPOKO, Academy of Sciences Moldova, R. JOHNSON, Department of Physics, Boston College, Chestnut Hill, MA 02467, M.J. GRAF, Department of Physics. Boston College. Chestnut Hill MA 02467 — Theoretical work based on one-dimensional (1D) models indicates that Bi wires with diameter smaller than 50 nm can exhibit superior thermoelectric properties since the density of states at the Fermi level of a 1D system can be tuned to very high values. Also, recently, angle-resolved photoemission spectroscopy (ARPES) studies of Bi thin films have shown that Bi nanowires support Rashba spin-orbit surface states, with high carrier densities of around $5 \times 10^{12}$ cm$^{-2}$, that are hybridized with “bulklike” electrons and holes, a phenomenon that has not been considered in current models of Bi nanowires. We carried out an experimental study of the transport properties and thermopower of bismuth nanowire arrays (NWA) with wire diameters ranging between 60 nm and 13 nm at temperatures ranging between 4 K and 300 K, for magnetic fields of up to 1 T. Both pure bismuth and doped Bi were studied. The results are interpreted in a multicarrier diffusion thermopower model.

1Supported by National Science Foundation and Army Research Office.

1:51PM J28.00014 Tuning the Thermoelectric Properties of Metal-Molecule-Metal Junctions, K. BAHETI, J.A. MALEN, P. DOAK, T.D. TILLEY, A. MAJUMDAR, R. SEGALMAN, Univ. of California, Berkeley — Thermoelectric materials have application in power generation and refrigeration, with several advantages over conventional power cycles including lack of moving parts, silent operation, miniaturization, and CO2 free conversion of heat to electricity. Nonetheless, low thermodynamic efficiency has limited their applicability. Here we examine a new class of inexpensive thermoelectric materials composed of organic-inorganic heterostructures. Thermopower measurements of 1,4-Benzenediethyl (BDT) molecule between Au electrodes, using a modified scanning tunneling microscope (STM), have been previously reported. This method is used to interrogate junctions where, the BDT molecule has been doped by the addition of substituent groups on the benzene ring. Our measurements show that we can tune the thermoelectric properties of such junctions in a controllable way by the addition of substituents. This in conjunction with a calculated transmission function imply a simultaneous increase in the thermopower and conductance, which has hitherto been impossible to attain in simple materials. We observe an increase of $\sim 50\%$ in the power factor, defined as $S^2\sigma$, of the junction upon substitution of electron donating groups in benzenediethyl. Hence, a ground up approach to building thermoelectric materials, from an endless array of possible organic-inorganic heterostructures, evokes hope for efficient thermoelectric energy conversion.

2:03PM J28.00015 Transport properties and the thermoelectric figure-of-merit of single molecule systems, PADRAIG MURPHY, Department of Physics, UC Berkeley, SUBROTO MUKERJEE, JOEL MOORE, Department of Physics, UC Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — The thermoelectric properties of molecules are both of fundamental interest and of interest for the construction of energy conversion devices. These transport properties are sensitive to interactions within the molecule, the hybridization energy between the molecular energy levels and the leads, and to the temperature. We present numerical and theoretical results on the conductance and thermopower, and discuss the parameter values for which the figure-of-merit, which parametrizes the efficiency of energy conversion devices, is optimal. The numerical results for the thermopower can be obtained at fixed particle number for finite systems using an appropriate generalization of the approach of Gogolin and Prokof'ev to electrical conductance.


11:15AM J29.00001 Biased bilayer graphene: Hall effect and zero-energy Edge States, NUNO PERES, University of Minho — We demonstrate that the electronic gap of a graphene bilayer can be controlled externally by applying a gate bias. From the magneto-transport data (Shubnikov-de Haas measurements of the cyclotron mass), and using a tight binding model, we extract the value of the gap as a function of the electronic density. We show that the gap can be changed from zero to mid-infrared energies by using fields of $\lesssim 1$ V/nm, below the electric breakdown of SiO$_2$. The opening of a gap is clearly seen in the quantum Hall regime. We further report the existence of zero energy surface states localized at zigzag edges of bilayer graphene. It is shown that zero energy edge states in bilayer graphene can be divided into two families: (i) states living only on a single plane, equivalent to surface states in monolayer graphene; (ii) states with finite amplitude over the two layers, with an enhanced penetration into the bulk.
11:51AM J29.00002 Cyclotron resonance in bilayer graphene, ERIK HENRIKSEN, Columbia University, ZHIGANG JIANG, LI-CHUN TUNG, NHMFL, MOLLIE SCHWARTZ, Columbia University, MAIKA TAKITA, Barnard College, YONG-JIE WANG, NHMFL, PHILIP KIM, HORST STORMER, Columbia University — The hyperbolic dispersion of bilayer graphene leads to a Landau level (LL) spectrum that is linear in the magnetic field, B, at low energies but shifts to a $\sqrt{B}$ dependence with increasing energy. Here we present the first infrared transmission measurements of the unique B-field dependence of LL transitions in bilayer graphene, in a gated 400$\mu$m$^2$ sample in fields up to $B = 18$ T. Eight intraband transitions are observed among LL indices $|n| \leq 4$, including the unusual zero-energy $n = 0$ level, and are found to follow a selection rule of $\Delta n = \pm 1$. We find the change in field dependence is plainly visible between the behavior of the transition energies for $n = -1 \rightarrow 0$ and $n = 0 \rightarrow +1$, which are close to linear in B, as compared with all other transitions which display a clear $\sqrt{B}$ behavior. However, the shift in field dependence occurs at energies well below where it is expected based on nearest-neighbor tight-binding calculations, and a single set of fitting parameters within this theory fails to describe our results.

12:03PM J29.00003 Graphene as an electronic membrane, EUN-AH KIM, Stanford University, ANTONIO CASTRO NETO, Boston University — Experiments are finally revealing intricate facts about graphene which go beyond the ideal picture of relativistic Dirac fermions in pristine two dimensional (2D) space, two years after its first isolation. While observations of rippling [1, 2, 3] added another dimension to the richness of the physics of graphene, scanning single electron transistor images displayed prevalent charge inhomogeneity [4]. The importance of understanding these non-ideal aspects cannot be overstated both from the fundamental research interest since graphene is a unique arena for their interplay, and from the device applications interest since the quality control is a key to applications. We investigate the membrane aspect of graphene and its impact on the electronic properties. We show that curvature generates spatially varying electrochemical potential. Further we show that the charge inhomogeneity in turn stabilizes ripple formation.[5]

12:15PM J29.00004 Demonstration of one-parameter scaling at the Dirac point in graphene, JENS H. BARDARSON, J. TWORZYDLO, P. BROUWER, C.W.J. BEENAKKER, Instituut-Lorentz, Universiteit Leiden — We numerically calculate the conductivity $\sigma$ of an undoped graphene sheet (size $L$) in the limit of vanishingly small lattice constant. We demonstrate one-parameter scaling for random impurity scattering and determine the scaling function $\partial T/L \sigma = -\partial L/L \sigma$. Contrary to a recent prediction, the scaling flow has no fixed point ($\beta > 0$) for conductivities up to and beyond the symplectic metal-insulator transition. Instead, the data supports an alternative scaling flow for which the conductivity at the Dirac point increases logarithmically with sample size in the absence of intervalley scattering — without reaching a scale-invariant limit.

12:27PM J29.00005 Electron localization in gapped bilayer graphenes with disorder, MIKITO KOSHINO, Columbia University, Tokyo Institute of Technology — The bilayer graphene is a zero-gap semiconductor, and it is known that the width of energy gap can be controlled by the electric field perpendicular to the layer [1,2]. Even in zero magnetic field, the electronic states carry the non-zero Hall conductivity in presence of the gap, while the Hall currents cancel out in summation over two valleys (K and K' points). Here we numerically calculate the electronic states in gapped bilayer graphenes with the smooth disorder potential, and estimate the localization length as a function of the gap width $\Delta$. We find that the conductivity at zero Fermi energy does not simply go down as $\Delta$ increases, but has a maximum at a certain finite $\Delta$, and the localization length diverges there. We show that this can be interpreted as a “Hall plateau transition” in each decoupled valley, even though the total Hall conductivity remains zero. [1] Meyer, J.C., et al., Nature 446, 60 (2007). [2] Stolyarov E. et al., PNAS, 104, 9209 (2007). [3] Ishigami, M. et al., Nano Letters 7, 1643 (2007). [4] Martin, J. et al., unpublished, cond-mat/0705.2180 (2007). [5] E.-A. Kim and A. Castro Neto, cond-mat/0702562

12:39PM J29.00006 Effect of electron interactions on the infrared conductivity of a monolayer graphene, M. M. FOGLER, L. M. ZHANG, UCSD — Recent experiments on the infrared spectroscopy of a monolayer graphene has revealed an unexpected non-Lorentzian form of the Drude peak and an anomalously large broadening of the interband absorption edge in this material. We present a theoretical investigation that attributes these features to Coulomb scattering between Dirac quasiparticles. This scattering shows up in the dynamical conductivity up to and beyond the symplectic metal-insulator transition. Instead, the data supports an alternative scaling flow for which the conductivity at the Dirac point increases logarithmically with sample size in the absence of intervalley scattering — without reaching a scale-invariant limit.

12:51PM J29.00007 Excitonic Effects in the Optical Spectra of Graphene Nanoribbons, LI YANG, MARVIN COHEN, STEVEN LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division of Lawrence Berkeley National Laboratory — We present a first-principles calculation of the optical properties of graphene nanoribbons (GNRs) with many-electron effects included, employing the GW-BSE approach. The reduced dimensionality of GNRs gives rise to an enhanced electron-hole binding energy for both bright and dark exciton states and changes the optical spectra significantly. The characteristics of the excitons of different types of GNRs are compared and discussed. The enhanced excitonic effects found here are expected to be of importance in considering possible applications (such as optoelectronics) of graphene-based nanostructures. This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by Datastar at the San Diego Supercomputer Center.

1:03PM J29.00008 Localized states at zigzag edges of graphene multilayers and graphite steps, EDUARDO V. CASTRO, J.M.B. LOPES DOS SANTOS, CFP and Departamento de Física, Faculdade de Ciências Universidade do Porto, Portugal, N.M.R. PERES, Center of Physics and Departamento de Física, Universidade do Minho, Portugal, F. GUINEA, Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, Spain, A. H. CASTRO NETO, Department of Physics, Boston University, USA — Among the uncommon features of graphene monolayer we find the presence of zero energy states localized at zigzag edges, leading to the self-doping phenomenon and inducing edge magnetization. Here we report the existence of zero energy surface states at zigzag edges of bilayer graphene and stacks with any number of layers. Working within the tight-binding approximation we derive an analytic solution for the wavefunctions of these peculiar surface states. It is shown that zero energy edge states in bilayer graphene can be divided into two families: (i) states living only on a single plane, equivalent to surface states in monolayer graphene; (ii) states with finite amplitude over the two layers, with an enhanced penetration into the bulk. The effect of edge states on the electronic structure and magnetic order of bilayer graphene nanoribbons is also studied. We show that edge states measured through scanning tunneling microscopy and spectroscopy of graphite step edges belong to family (i) or (ii) mentioned above, depending on the way the top layer is cut.
1:15PM J29.00009 Minimal conductivity of graphene: role of the Coulomb interaction, VLADIMIR JURICIC, IGOR F. HERBUT, Department of Physics, Simon Fraser University, Canada. OSKAR VAPEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University, USA — The effect of the Coulomb interaction on the zero-temperature low-frequency conductivity in undoped graphene is studied. We will show that the Coulomb interaction introduces a universal and positive leading logarithmic correction to the gaussian value of the dc conductivity [1]. This finding suggests that the origin of the unusually large minimal conductivity observed in graphene may be intrinsic, and arises from the Coulomb correction effectively cut off by finite temperature/disorder/size effects. A mechanism of such a cutoff based on the non-trivial interplay between the Coulomb interaction and the ripples, both unavoidably present in the graphene sheet, will be briefly discussed. References: [1] I. F. Herbut, V. Juricic, and O. Vafek, arXiv:0707.4171.

1:27PM J29.00010 Low density ferromagnetism in a biased bilayer graphene, TOBIAS STAUBER, Instituto de Ciencia de Materiales de Madrid (CSIC), EDUARDO CASTRO, CFP and Departamento de Física, Facultade de Ciencias Universidade do Porto, NUNO PERES, NUNO SILVA, Centro de Física e Departamento de Física, Universidade do Minho — We compute the phase diagram of a biased graphene bilayer. The existence of a ferromagnetic phase is discussed with respect both to carrier density and temperature. We find that the ferromagnetic transition is first order, lowering the value of $U$ relatively to the usual Stoner criterion. We show that in the ferromagnetic phase the two planes have unequal magnetization and that the electronic density is hole like in one plane and electron like in the other.

1:39PM J29.00011 Minimal conductivity of rippled graphene with topological disorder, ALBERTO CORTIJO, MARIA VOZMEDIANO, Instituto de Ciencia de Materiales de Madrid-CSIC — We study the transport properties of a neutral graphene sheet with curved wrinkles induced or stabilized by topological defects. The proposed model gives rise to Dirac fermions in a random magnetic field and a random space dependent Fermi velocity induced by the curvature. This last term leads to singular long range correlated disorder with special characteristics. The Drude minimal conductivity at zero energy is found to be inversely proportional to the density of topological disorder, a signature of diffusive behavior.

1:51PM J29.00012 Weak Localization of Dirac Fermions in Graphene, XIN-ZHONG YAN, C. S. TING, TCS, University of Houston — In the presence of the charged impurities with screened Coulomb potentials, we study the weak localization (WL) effect by evaluating the quantum interference correction (QIC) to the conductivity of Dirac fermions in graphene. With the inelastic scattering rate due to electron-electron interactions obtained from our previous calculation, we investigate the dependence of QIC on the carrier concentration, the temperature and the size of the sample. It is found that WL is present in large size samples at finite temperature while the strength of the intervalley scatterings due to the charged impurities is not weak. In addition, we argue that the system is delocalized at very low doping. We also analyze the absence of WL in experiment. It is found that WL is quenched at low temperature for small size samples as studied in the experiments.

2:03PM J29.00013 Electric Transport Theory of Dirac Fermions, YOUSEF ROMIAHI, Department of Physics, University of Houston, TX. 77204 and Texas Center for Superconductivity, University of Houston, TX. 77204, XIN-ZHONG YAN, Chinese Academy of Sciences, P. O. Box 603, Beijing 100080, China, CHIN-SEN TING, Department of Physics, University of Houston, TX. 77204 and Texas Center for Superconductivity, University of Houston, TX. 77204 — The self-consistent Born approximation is employed to calculate transport properties in graphene with finite-range impurity potentials. The current-current correlation function is determined by a system of four coupled integral equations, unlike the case of short-range impurity scattering, and yet the results for the latter can exactly be reproduced in our formalism. As a test, we numerically calculate the dc electric conductivity of graphene for charged impurities with screened Coulomb potential, the linear dependence of the dc conductivity on the carrier concentration and the extrapolated value for zero-doping is shown to be finite, in a qualitative agreement with the experimental observations.

Tuesday, March 11, 2008 11:15AM - 2:15PM
Session J30 DMP: Optical Properties and Experimental Characterization of Graphene and Related Structures — Morial Convention Center 222

11:15AM J30.00001 Photo-induced structural dynamics of graphitic carbon studied by ultrafast electron nanocrystallography, RAMANI K. RAMAN, YOSHIE MUROOKA, RYAN A. MURDICK, CHONG-YU RUAN, Michigan State University — We report the studies of photo-induced structural dynamics of graphite and multi-wall carbon nanotubes (MWCNT) using ultrafast electron nanocrystallography. Graphite, upon excitation, contracts along its c-axis causing a reduction of the interlayer distance, which is the first step towards diamondization. MWCNT on the other hand, display an energy-dependent electron-phonon coupling mechanism. Upon excitation at 400nm, the promoted carriers can transfer their excess energy to the lattice rapidly within 5-10 ps whereas at 800nm it takes around 20-30ps for the same. This indicates a more efficient electron-phonon coupling at 400nm where the excited carriers are more strongly coupled to the lattice. Both graphite and MWCNT also exhibit a transient photovoltaic effect where an accumulation of excited charge carriers at the sample interface causes a collective shift of the Bragg peaks. We found that the charge dynamics and atom dynamics are intimately correlated at interfaces.

11:27AM J30.00002 Non-destructive optical characterization of DNA-wrapping of single-walled carbon nanotubes, S. E. SNYDER, S.V. ROTKIN, Lehigh University — Single-stranded DNA can form a stable hybrid structure with a single-walled carbon nanotube, allowing dispersion of individual nanotubes in aqueous solution and facilitating the development of methods to separate nanotubes by type. Optical and electronic properties of specific DNA-nanotube structures are the focus of our study due to potential optoelectronic device applications. Within a semi-empirical tight-binding approach, we have studied changes in optical absorption of a single-walled carbon nanotube resulting from a helical wrap of ionized single-stranded DNA. The one-electron absorption spectrum for light polarized across the tube is sensitive to bandstructure modulation due to the wrapping. For a non-chiral tube, the helical perturbation generates “natural” optical activity in the DNA-nanotube complex, yielding circular dichroism. Symmetry breaking due to the Coulomb interaction and the ripples, both unavoidably present in the graphene sheet, will be briefly discussed. References: [1] I. F. Herbut, V. Juricic, and O. Vafek, arXiv:0707.4171.
11:39 AM J30.00003 Incommensurately Stacked Graphene Bi-Layer: A Raman Scattering Study\textsuperscript{1}. AWNISH GUPTA, Y. TANG, T. RUSSIN, V. CRESPI, P. EKLUND, Pennsylvania State University — We report results of Raman scattering studies of two novel graphene systems based on incommensurate stacking of sp\textsuperscript{2} carbon: (1) an incommensurate bi-layer (IBL) formed by folding a graphene sheet onto itself; (2) a graphene scroll formed by rolling up a graphene sheet via a shearing motion between scotch tape and substrate during the micro-mechanical cleaving process. In (1), we have a flat bi-layer system; in (2) it is a gently curved multilayer system — both should be incommensurate. Interestingly, although no significant D-band is observed in the parent graphene sheet, the incommensurate contact of the graphene sheet in (1) and (2) leads to strong D-band scattering near 1350 cm\textsuperscript{-1} using 514.5 nm excitation. The dispersion of the D-bands in (1) and (2) is significantly different: scroll (~38 cm\textsuperscript{-1}/eV) and IBL (~50 cm\textsuperscript{-1}/eV). A second Raman band is observed nearby at ~1384 cm\textsuperscript{-1} in both the IBL and the scroll. However, the ~1384 cm\textsuperscript{-1} band is non-dispersive in both cases and is much sharper in the IBL than in the scroll. Our data will be compared to theoretical calculations based on double-resonant (DR) scattering and the electronic states of an IBL.

\textsuperscript{1} NSF-ECS0609243

11:51 AM J30.00004 Anharmonic Effects in Raman Scattering Few-Layer Graphene System\textsuperscript{1}. TIMOTHY RUSSIN, Pennsylvania State University, AWNISH GUPTA, PETER EKLUND — Result of Raman scattering studies from supported and suspended n-layer graphene films (nGLs) are presented for the temperature range of ~190 to 500 °C. The samples were either supported directly on a Si/SiO\textsubscript{2} substrate or suspended over lithographically produced trenches; the measurements were performed in a N\textsubscript{2} atmosphere. For both supported and suspended films, the magnitude of the negative temperature coefficient of the G-band frequency (cm\textsuperscript{-1}/K) is found to decrease with increase in number of layers n in the nGL films (i.e., supported 1GL, 2GL and 5GL show ~0.10, ~0.13, and ~0.28 cm\textsuperscript{-1}/K, respectively.) The anharmonic coefficients are significantly higher than for highly oriented pyrolytic graphite (HOPG). Surprisingly, the G-band linewidth increases with temperature for the supported films and decreases with temperature for the suspended films. Furthermore, we see evidence for a permanent morphological change at ~300 °C for supported nGLs via new D-band and D’-band scattering. Unsupported films exhibit these changes at higher temperatures. The mechanism and details of the irreversible morphological change(s) is not yet known.

\textsuperscript{1} NSF-ECS0609243

12:03 PM J30.00005 Tunneling spectroscopy of single- and double-layer graphene planar tunnel junctions. CONOR PULS, NEAL STALEY, YING LIU, Department of Physics, Pennsylvania State University — It is of fundamental as well as technological concern if there exists an energy gap in single- and double-layer graphene devices. Single-layer graphene is thought to be gapless while double-layer graphene features an energy gap tunable by controlling the charge difference between the two layers. Previously, scanning tunneling microscopy and spectroscopy studies have been employed to examine energy spectra of graphene films. This approach produces local charge inhomogeneity at the probe tip that could significantly alter the local density of states (DOS) in graphene. Planar tunnel junctions provide a probe of the DOS that should not induce such an inhomogeneity in the charge carrier density. We fabricated planar tunnel junctions on single- and double-layer graphene using an ultrathin quartz filament as a shadow mask over mechanically exfoliated graphene as an alternative to lithographic procedures so as to avoid possible contamination in a wet lithography process. We have measured tunneling spectra for both weakly and strongly disordered samples. For single-layer graphene, we observed an unexpected gap. For double-layer graphene, we found a gap and other features in the tunnel spectra by changing the back gate and tunnel junction bias voltages independently — thereby tuning the charge difference between the top and bottom layer — as well as varying magnetic field and temperature.

12:15 PM J30.00006 The G* (2450 cm\textsuperscript{-1}) Double Resonance Raman Peak in single-, few-layer graphene and DWNTs, ALFONSO REINA, HYUNGBIN SON, FEDERICO VILLALPANDO-PAEZ, HOOTAN FARHAT, JING KONG, MIT, MILDELD DRESSELHAUS, MATERIALS SCIENCE AND ENGINEERING TEAM, ELECTRICAL ENGINEERING AND COMPUTER SCIENCE TEAM, PHYSICS TEAM, IIC, BERKELEY TEAM — The dispersion and skewness of the 2450 cm\textsuperscript{-1} peak in the raman spectra of carbon structures was analyzed. The dispersion of this peak for graphene is smaller in extent and of opposite sign than that for the G* (~2700 cm\textsuperscript{-1}). This dispersion is independent on number of layers. The peak shows asymmetry (skewness) which increases with $E_{\text{laser}}$. The observations can be explained by viewing this double resonance process arising by the scattering with both an iT0 and a iLA phonon. The peak becomes more symmetric in DWNTs and it shows a stronger curvature dependence than the G* peak.

12:27 PM J30.00007 Probing Non-equilibrium Phonon Dynamics in Graphite by Time-Resolved Raman Spectroscopy, HUGEN YAN, Columbia University, DAOHUA SONG, KIN FAI MAK, IOANNIS CHATZAKIS, JANINA MAULTZSCH, TONY HEINZ — Time-resolved Raman spectroscopy has been applied to obtain direct information about phonon lifetimes in graphite. A non-equilibrium population of zone-center optical phonons was produced by the rapid relaxation of charge carriers following photoexcitation of the sample with a femtosecond laser pulse. The subsequent evolution of the phonon population was recorded using the strength of G-mode anti-Stokes Raman scattering from a time-delayed femtosecond probe pulse. A population lifetime for the G-mode phonons of approximately 2 ps was found. Analogous measurements of optical-phonon lifetimes were also conducted in few-layer graphene samples produced by mechanical exfoliation of bulk graphite. Results obtained for graphite and few-layer graphene will be compared with one another, as well as with earlier data on the lifetime of G-mode phonons in single-walled carbon nanotubes [1].


12:39 PM J30.00008 Transfer of Graphene to Alternative Substrates\textsuperscript{1}. TRACY MOORE, J.H. CHEN, D.R. HINES, E.D. WILLIAMS, University of Maryland, J. SIMSPON, A.R.H. WALKER, NIST — Graphene transport properties are limited by charge defects in SiO\textsubscript{2}, and by large charge density due strong interaction with SIC. We have investigated the transfer of graphene from one substrate to another using high pressures and temperatures to achieve control of the substrate interactions and thus their effects on graphene. The direct transfer from HOPG to alternative substrates PET and PMMA yields mostly multilayer, opaque graphite flakes. Raman signatures of the thinner, translucent flakes on PMMA can be clearly distinguished from the PMMA spectra and show a downshift in the G’ peak that occurs around 2700 cm\textsuperscript{-1} and a relative intensity of G to G’ peak of approximately one; characteristics of graphene spectra. In addition the transfer from SiO\textsubscript{2} to alternative substrates occurs readily for PET substrates, and infrequently for PMMA substrates with thicker flakes transferring more readily than thin flakes. Graphene transfer from 1) direct HOPG, 2) flakes on SiO\textsubscript{2}, and 3) the possibility of direct transfer from epitaxial graphene on SiC will be presented, along with the resulting device characteristics.

\textsuperscript{1} Supported by the Laboratory for Physical Sciences and NSF-MRSEC at UMD
12:51PM J30.00009 Gap and Impurity induced states on graphene layers, CHANYONG HWANG, DOHYUN LEE, WON DONG KIM, Korea Research Institute of Standards and Science, JUNGHWA YANG, JISANG HONG, Department of Physics, Pukyong National University — One of the interesting phenomena in graphene is the linear Fermi level crossing at the Dirac point. For the measurement of electronic structure, few layers of graphenes are formed on top of SiC substrate by thermal treatment. As the thickness of graphene layers increases, the formation of the gap near Dirac point is somewhat controversial. Recently this gap has been demonstrated to be tunable by the electric field. We have used angle-resolved photoemission spectroscopy and STM to characterize this gap state and actual morphology of the graphene layers to clarify this controversial issue. In addition, we have shown that the adatom carbon can play an important role in gap state. First principles calculation on this carbon adatom state will be discussed.

1:03PM J30.00010 Single Layer Graphene formation on Silicon Oxide surface(001), HEE SUNG CHOI, YOUNG-KYUN KWON, University of Massachusetts Lowell — Recently graphene is one of most interesting topics in physics and other research fields. For future nanoelectronics applications, graphene formation becomes an important issue. Here we present our theoretical study of how to make a graphene layer on silicon oxide surfaces. In this work, density functional theory calculations are used to determine atomic structures and energies for graphene formation from various carbon sources, such as anthracene, on silicon oxide. We will also present optimal graphene formation conditions obtained from our ab initio molecular dynamics simulations.

1:15PM J30.00011 Soldering to a single atomic layer, CAGLAR GIRIT, ALEX ZETTL, UC Berkeley, LBNL — The standard technique to make electrical contact to nanostructures is electron beam lithography. This method has several drawbacks including complexity, cost, and sample contamination. We present a simple technique to cleanly solder submicron sized, Ohmic contacts to nanostructures. To demonstrate, we contact graphene, a single atomic layer of carbon, and investigate low- and high-bias electronic transport. We set lower bounds on the current carrying capacity of graphene. A simple model allows us to obtain device characteristics such as mobility, minimum conductance, and contact resistance.

1:27PM J30.00012 Synthesis of Carbon Nanotubes by Rolling Up Patterned Graphene Nanoribbons Using Selective Atomic Adsorption1, DECAI YU, FENG LIU, University of Utah, LIU TEAM — We demonstrate a new method for synthesizing Carbon Nanotubes (CNTs), using first principles and classical molecular dynamics simulations. The single-walled nanotubes (SWNTs) are formed by rolling up graphene nanoribbons patterned on graphite films, through adsorption of atoms of varying coverage, which introduces an external stress to drive the folding process. The diameter and chirality of SWNTs can be a priori controlled by patterning graphene nanoribbons with predefined width and direction, so that the post-synthesis sorting process is eliminated. Our method allows potentially mass production of identical tubes and easy integration into device structures on a substrate.

1We acknowledge support from DOE.

1:39PM J30.00013 13C NMR studies on the organic zero-gap system, \( \theta-(BEDT-TTF)_2I_3 \) under pressure, KAZUYA MIYAGAWA, University of Tokyo and JST-CREST, MÔTOAI HIRAYAMA, University of Tokyo, MASAFUMI TAMURA, RIKEN, KAZUSHI KANODA, University of Tokyo and JST-CREST. — We present NMR data for the organic material, \( \theta-(BEDT-TTF)_2I_3 \) under pressure, which is a candidate for zero-gap conductor with cone-like dispersion. The quasi-two-dimensional organic conductor \( \alpha-(BEDT-TTF)_2I_3 \) is known to show peculiar behaviors under high pressure. The resistivity is insensitive to temperature, while the Hall coefficient is strongly dependent on temperature. The band calculation suggests that this system is in the zero gap state with a linear dispersion around the Fermi energy. While the \( \theta-(BEDT-TTF)_2I_3 \) is metallic under ambient pressure, above 5 kbar temperature dependences of resistivity and Hall coefficient are similar to those of \( \alpha-(BEDT-TTF)_2I_3 \). It is remarkable that the graphite like zero-gap state is realized in a bulk system. We have performed preliminary investigation into the magnetism of \( \theta-(BEDT-TTF)_2I_3 \) under 8 kbar by \(^{13}\)C NMR. The external field is applied to parallel to the conducting layer. In constant to the simple metallic behavior observed under ambient pressure (Korriga's relation holds), the Knight shift vanishes in proportion with temperature and 1/\( T \).

1:51PM J30.00014 UHV Growth of Graphene on SiC, PAUL CAMPBELL, GLENN JERNIGAN, KEITH PERKINS, BRENDÁ VANILÍN, RACHEL MYERS-WARD, KURT GASKILL, JAMES CULBERTSON, JEREMY ROBINSON, ERIC SNOW, Naval Research Laboratory — We report growth of graphene on Si- and C-face semi-insulating 6H SiC in UHV by thermal Si desorption/reconstruction of the remaining C. The SiC was etched in H₂ up to 1500 °C to smooth the surface. XPS shows the H₂-etched surfaces are covered by an oxide which desorbs at 1000 °C, resulting in a surface containing excess Si. At 1300 °C, the surface becomes stoichiometric in Si and C and a \( \sqrt{3} \times \sqrt{3} \) R30 LEED pattern is observed. At 1350 °C, we observe a 6/\( \sqrt{3} \) x 6/\( \sqrt{3} \) R30 LEED pattern when the graphene has formed, and a 1x1 LEED pattern for graphite films formed at temperatures greater than 1400 °C. Graphene layers were grown under a variety of temperatures and conditions and characterized using XPS, LEED, AFM, Raman spectroscopy, and Hall effect. Top-gated FETs were fabricated with a wide range of gate lengths (1-25 microns) and gate widths (2-130 microns), and transistor operation was obtained for both single and multiple graphene layers.

1Supported by NRL Institute for Nanoscience
2ASEE postdoctoral Associate
3ASEE Postdoctoral Associate
4NRC Postdoctoral Associate

2:03PM J30.00015 UHV electron-probing of micro-mechanically cleaved Graphene on SiO₂, K.R. KNOX, S. WANG, P. KIM, R.M. OSGOOD, Columbia University, T.O. MENTES, M.A.N ORTI, A. LOCATELLI, Elettra Trieste Italy, D. CVETKO, A. MORGANTE, TASC-INFN Trieste Italy — While graphene’s distinctive Dirac-cone electronic structure and simple 2D atomic structure have attracted major interest in the physics community, the inherent limitations of isolated graphene samples mounted on an insulating substrates have made it difficult to study such systems with typical UHV probes such as photoemission and low energy electron diffraction (LEED). While most single layer graphene transport measurements are done on micro-mechanically extracted samples on SiO₂, all photoemission and LEED measurements of graphene performed so far have used films grown on SiC substrates. In this talk, we will discuss the first results of UHV probes carried out exfoliated graphene bonded to SiO₂. Using the high spatial resolution of the nanospectroscopy beamline at the ELETTRA synchrotron light source, we have been able to overcome the size limitations, which have prevented previous UHV study of this system. We will discuss the results of our X-ray photoemission (XPS), UV photoemission (UPS) and LEED measurements on single and multilayer graphene samples.

Tuesday, March 11, 2008 11:15AM - 2:15PM –
Session J31 DMP DCOMP: Focus Session: Computational Nanoscience IV: Nanocrystals
Morial Convention Center 223
11:15AM J31.00001 Atomic design of semiconductor nanostructures with optimal thermoelectric properties

GIULIA GALLI, University of California Davis — The search for novel materials with optimal thermoelectric properties (for either thermoelectric power generation or heat dissipation) is an active field of research. We present atomistic and ab-initio simulations of selected nanomaterials, aimed at predicting thermal conductivities and electronic transport properties, and ultimately at designing materials with optimal thermoelectric figure of merit. In particular we focus on carbon nanotubes [1], silicon wires [2] and nanoporous silicon [3] and we discuss both strategies and algorithms to optimize thermoelectric properties at the nanoscale.


1Supported by DARPA grant # W911NF-06-1-0175.

11:51AM J31.00002 Ab initio method for the electron-phonon scattering times in semiconducting nanomaterials

NATHALIE VAST, JELENA SJAKSTE, Ecole Polytechnique, Laboratoire des Solides Irradiés, CEA-DSM-DRECAM, CNRS, 91128 Palaiseau, France, VALERIY TYUTEREV, Tomsk State Pedagogical University, Tomsk, Russia — The interaction of excited electrons with phonons plays a central role for electronic and transport properties at the nanoscale. It is the dominant process limiting the excitation lifetime at medium excitation energies. Despite its importance, a reliable approach within ab initio methods for phonon interaction with excited carriers was still lacking. We present in this work our fully ab initio approach to calculate the electron-phonon scattering times for collisions of carriers in the conduction band with short-wavelength phonons. We apply it to the deexcitation of hot electrons in GaAs [1,2], and to the lifetime of the direct exciton in GaP and GaAs [2,3], all in excellent agreement with experiments. Finally, we discuss the effect of nanostructuring on the electron-phonon coupling constants in GaAs/AlAs superlattices.


12:03PM J31.00003 Quantum-size-induced phase transitions in quantum dots: Indirect-band gap GaAs nanoostructures

ALEX ZUNGER, JUN-WEI LUO, ALBERTO FRANCESCHETTI, National Renewable Energy Lab — Quantum nanostuctures are often advertised as having stronger absorption than the bulk material from which they are made, to the potential benefit of nanotechnology. However, nanostuctures made of direct gap materials such as GaAs can convert to indirect-gap, weakly-absorbing systems when the quantum size becomes small. This is the case for spherical GaAs dots of radius 15 Å or less (about 1000 atoms) embedded in a wide-gap matrix. The nature of the transition: Γ-to-X or Γ-to-L is however, controversial. The distinction can not be made on the basis of electronic structure techniques that misrepresent the magnitude of the various competing effective masses (e.g. DDA vs. GGA) or wavefunction coupling (e.g. tight-binding). Using a carefully fit screened pseudopotential method we show that the transition occurs from Γ to X, and, more importantly, that the transition involves a finite V (Γ-X) interband coupling, manifested as an “anti-crossing” between the confined electron states of GaAs as the dot size crosses 15 Å. The physics of this reciprocal-space Γ-X transition, as well as the real-space (type II) transition in GaAs/AlGaAs will be briefly discussed.

12:15PM J31.00004 Co-doping of Boron and Phosphorus in Silicon Nanoclusters

JAE-HYEON EOM, TZU-LIANG CHAN, JAMES R. CHELIKOWSKY, University of Texas at Austin — The effect of cluster size on the interaction between impurity atoms is studied using the first-principles calculations, i.e. pseudopotentials in real space. We calculate the stable configurations of B and P co-doped silicon nanoclusters as a function of size. We evaluate the evolution of interactions between impurity atoms by comparing the stable configurations. The evolution of photoluminescence is discussed.

12:27PM J31.00005 Quantum Confinement and Non-Magnetic-Doped Dilute Magnetic Semiconductors

HYUNWOOK KWAK, University of Minnesota, TZU-LIANG CHAN, JAMES R. CHELIKOWSKY, University of Texas — Dilute magnetic semiconductors are of interest for their unique magnetic properties and their promising role in development of “spintronic” semiconductor devices. Recently, a new dimension has been brought to this class of material by observing room temperature ferromagnetism in non-magnetic doped semiconductors and insulators. Using real-space pseudopotential applied to nitrogen-doped ZnO nanowires and nanocrystals, we report the theoretical evidence of magnetism in spatially confined non-magnetic doped semiconductor nanocrystals. Detailed electronic structures and magnetic properties are examined by comparing the total energy of different spin orderings and defect configurations. Besides the prediction of high Curie temperature, our results show that the ferromagnetic order becomes more stable when the nitrogen defects experience strong quantum confinement.

1This work was supported in part by the National Science Foundation under DMR-0551195 and the Department of Energy under DE-FG02-06ER15760 and DE-FG02-06ER46286.

12:39PM J31.00006 Impurity Doping in PbSe Nanocrystals

STEVEN ERWIN, Naval Research Laboratory — We recently proposed that impurity doping in colloidal grown nanocrystals is controlled primarily by kinetics, rather than by thermodynamics. In this “trapped dopant” model, the diffusion of an impurity through a nanocrystal is negligible at colloidal growth temperatures. Therefore, an impurity can only be incorporated into a growing nanocrystal if it first adsorbs on the surface and is then overgrown. But this simple surface adsorption process is complicated by a competing “anti-crossing” between the confined electron states of GaAs as the dot size crosses 15 Å. The physics of this reciprocal-space Γ-X transition, as well as the real-space (type II) transition in GaAs/AlAs will be briefly discussed.


12:51PM J31.00007 Size Limits on Doping Phosphorous into Silicon Nanocrystals

TZU-LIANG CHAN, MURILLO L. TIAGO, University of Texas at Austin, EPFTHIMOS KAXIRAS, Harvard University, JAMES R. CHELIKOWSKY, University of Texas at Austin — The evolution of the semiconductor industry requires continued miniaturization. As this trend continues, devices will ultimately approach the nanometer-scale and it is expected that device construction based on macroscopic laws will start to fail. Using a real-space first-principles pseudopotential method, we study doping in the nano-regime using phosphorus-doped Si nanocrystals as the prototypical system. We simulate phosphorus-doped Si nanocrystals with diameter up to 6 nm and study the evolution of the defect state with the size of the nanocrystal. Our calculated size dependence of hyperfine splitting is in excellent agreement with experimental data. The effect of quantum confinement is also manifested in the higher binding energy of the dopant electron, we estimate that phosphorus in Si nanocrystals of less than 20 nm in diameter will not be a shallow donor. We also find that for Si nanocrystals smaller than 2 nm in diameter, the phosphorus atom will be energetically expelled to the surface, leading to a self-purification mechanism that hinders the incorporation of impurity atoms into nanocrystals.

1This work was supported in part by the National Science Foundation under DMR-0551195.
1:03PM J31.00008 Interface chemistry of silicon nanocrystals embedded in silica\(^1\). DUNDAR YILMAZ, CEYHUN BULUTAY, Bilkent University, TAHIR CAGIN, Texas A&M University — Molecular dynamics simulations of realistic-sized silicon nanocrystals (NCs) with the diameters in the range from 1 nm to 3 nm embedded in amorphous oxide are carried out till steady state conditions with the chemical environment described by the reactive force field model. We identify different types of three-coordinated oxygen (3cO) complexes, previously not noted, on the oxide interface. No double bonds were observed. We reveal that the interface bond topology evolves among different oxygen bridges through these 3cO complexes. The abundance and the charge distribution of each oxygen complex is determined as a function of the NC size as well as the transitions among them. The number of bridge bonds is observed to scale with surface area, thus the curvature has a small effect on the number of bridges. Among the three bonds of 3cO, the weaker bond is more susceptible to bond breaking which is also likely to take part in an optical activity through bond breaking and reformation. Our results indicate that the Si NC-oxide interface is more complicated than the previously proposed schemes which were based on solely double and bridge bonds.

\(^1\)Supported by Turkish Scientific and Technical Council TUBITAK with the Project No. 106T048 and BIDEB-2221 Programme.

1:15PM J31.00009 Structure and electronic properties of gold-tipped CdSe nanorods\(^1\). N. BARNETT, UZI LANDMAN, Georgia Institute of Technology — We investigate CdSe nanorods capped by gold contacts and passivated by phospho-organic molecules of varying chain length. The geometry is optimized and the electronic structure obtained using first-principles quantum mechanical methods. We discuss the formation of Schottky barriers, the development of interfacial dipoles, the presence and extent of gap states induced by the metallic contact and of states in the semiconductor energy gap associated with the passivant carbon chains.

\(^1\)Computations performed at the National Center for Computational Sciences

1:27PM J31.00010 Förster resonant energy transfer between CdSe nanocrystals: An empirical pseudopotential/transition density cube approach\(^2\). JOSHUA SCHRIER, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We study the energy transfer between semiconductor nanocrystal dots and rods of CdSe using a semiempirical pseudopotential method (SEPM) description of the electronic structure of the nanocrystals, followed by evaluation of the Coulombic contribution to the energy transfer evaluated using the transition density cube (TDC) method. Our results are compared to the dipole-dipole theory of Förster to characterize the effects of nanocrystal shape, distance, and orientation. In agreement with previous effective-mass and tight-binding studies, we find that the coupling between spherical nanocrystals is well described by the Förster model. In contrast, we find that rod-shaped nanocrystals display more complicated behavior, which may be relevant to exciton migration in all-inorganic nanorod-based photovoltaic devices.

\(^2\)This work was supported by U.S. Department of Energy under Contract No.DE-AC02-05CH11231 and used the resources of the National Energy Research Scientific Computing Center.

1:39PM J31.00011 Polar properties of ZnO nanostructures. GIANCARLO CICERO, Politecnico of Torino, Torino, Italy; CNR-IMEM, Parma, Italy, ANDREA FERRETTI, CNR-S3, Modena, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy — The advent of all-inorganic nanorod-based photovoltaic devices critically enhances the role of surface and interface effects on bulk properties and determines the physical characteristics of the material: in particular, the understanding of the electronic properties of nanosized structures requires a proper accurate treatment. Here we report on first principles density functional calculations of the structural and electronic properties of the (1-100) “non-polar” surface of hexagonal zinc oxide (ZnO) and compare the results with those of ZnO nanowires grown along the [0001] direction and analogous exposed cuts, with a diameter range of about 9-23 Å. We discuss the formation of Schottky barriers, the development of interfacial dipoles, the presence and extent of gap states induced by the metallic contact and of states in the semiconductor energy gap associated with the passivant carbon chains.

1:51PM J31.00012 Softening of ultra-nanocrystalline diamond at small grain sizes, GEORGIOS KOPIDAKIS, Department of Materials Science and Technology, University of Crete, IOANNIS REMEDIAKIS, Department of Materials Science and Technology and Department of Physics, University of Crete, PANTELIS KELIRES, Department of Physics, University of Crete and Dept. of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology — Ultra-nanocrystalline diamond is a polycrystalline material, having crystalline diamond grains of sizes in the nanometer regime. We study the structure and mechanical properties of this material as a function of the average grain size, employing atomistic simulations. Using the bulk and Young’s moduli as probes of stiffness, we observe softening of the material as the size of its grains decreases, similar to the reverse Hall-Petch effect observed for nanocrystalline metals. This softening is attributed to the enhanced fraction of interfacial atoms. The calculated scaling of the cohesive energy and bulk modulus with respect to average grain size agrees very well with this picture. Our results suggest that softening at very small grain sizes might be a generic property of nanocrystalline materials.

2:03PM J31.00013 A Molecular Dynamics Study of the Melting and Nucleation of Iron Nanoparticles YASUSHI SHIBUTA, TOSHIO SUZUKI, Department of Materials Engineering, The University of Tokyo — The melting and nucleation of iron nanoparticles were investigated by molecular dynamics simulation using a Finnis-Sinclair potential. The nanoparticle of the bcc single-crystal was uniformly melted from the surface at a melting point during heating, whereas a nucleus was generated near one side of an undercooled liquid droplet and the solidification spread toward another side at a lower temperature during cooling. The melting point and nucleation temperature decreased with particle radius. Moreover, the solid-liquid interfacial energy was estimated to be 0.101 J/m\(^2\) using a Gibbs-Thomson equation, which is of the same order as the experimental value based on Turnbull-Fusher’s classical nucleation theory.
11:15AM J32.00001 Spin-orbit damping in transition metals, KEITH GILMORE, National Institute of Standards and Technology — Magnetization dynamics are routinely described with the Landau-Lifshitz-Gilbert (LLG) equation. However, it is expected that the LLG equation fails to properly describe the large amplitude dynamics that occur during magnetization reversal. Improving switching speeds in nanoscale devices by tailoring materials requires both a qualitative understanding of the relaxation processes that contribute to damping and the ability to quantitatively calculate the resulting damping rates. We consider small amplitude LLG damping in transition metals as a prelude to approaching the more complicated mechanisms expected in complete reversal events. LLG damping rates in pure transition metal systems have been assessed using magnetization reversal data, including spin-pumping picture of the Gilbert damping. We also make contact with earlier theories of the transverse spin susceptibilities and with the conductivity, which can be calculated straightforwardly (no vertex corrections involved) leading to a Drude-like formula in which the inverses of the disorder and interaction scattering times enter in a simple additive form.


11:51AM J32.00002 Non-local damping effects in Py-Cu-FeMn trilayers, ERIC R.J. EDWARDS, LEI WEN, ZEENATH REDDY TADISINA, CLAUDIA K.A. MEWES, SUBHADRA GUPTA, TIM MEWES, Center for Materials for Information Technology, University of Alabama — We report a non-local enhancement of the Gilbert damping in Py-Cu-FeMn trilayers for in-plane ferromagnetic resonance measurements. We observe a 1/α dependence, t being the thickness of the permalloy, of the slope of the linewidth vs. frequency measurements indicating non-local contributions to the damping. In view of experimental verification of the adiabatic spin pump theory [1] in ferromagnetic heterostructures [2], these results suggest parallels in exchange biased systems. With the thickness of the non-magnetic layer, Cu, fixed below its spin-diffusion length, we understand this effect to be non-local resulting from the injection of spins by the precessing magnetization at the Py-Cu interface and subsequent scattering at the Cu-FeMn interface.


12:03PM J32.00003 Gilbert Damping in Single-Crystalline Ni/MgO(001)1, KEVIN J. SMITH, R. ALE LUKASZEW, ANNE REILLY, Department of Physics, College of William and Mary, GÜNTER LÜPKE, Department of Applied Science, College of William and Mary — The dynamical properties of Nickel and Nickel alloys are of great interest in spintronic applications, as these materials exhibit low coercivity and significant magnetoresistance, however, the interplay of the various damping mechanisms, such as two magnon scattering and local resonance, is not well understood. The frequency, ω, and Gilbert damping, α, behavior of uniform spin precession on Ni/MgO(001) are studied over a wide range of external field angles and magnitudes using the Time-Resolved Magneto-Optical Kerr effect (TR-MOKE). The damping parameter shows a strong dependence on the magnetocrystalline anisotropy, suggesting a tuneability of α over the range of 0.09 to 0.5. Two separate trends in α vs. ω are observed depending on the magnitude of the applied field when applied in-plane, indicating the presence of competing damping mechanisms. We further investigate these properties in measurements in which the external field is applied normal to the sample plane, thereby minimizing the role of two magnon scattering.

1Financial support provided by the National Science Foundation through grant DMR-0605661.

12:15PM J32.00004 Inhomogeneous Gilbert damping from disorder and electron-electron interactions1, Ewelina Hankiewicz, Fordham University, Giovanni Vignale, University of Missouri-Columbia, Yaroslav Tserkovnyak, University of California Los Angeles — We present a unified theory of Gilbert damping in itinerant ferromagnets at order α2 (α being the wave vector of the spin modulation) including electron-electron interactions and electron-impurity scattering – the idea being that these interactions are much stronger than the spin-orbit interaction, which controls the damping in the homogeneous case (α = 0). We show that Gilbert damping can be expressed in terms of the spin conductivity, which can be calculated straightforwardly (no vertex corrections involved) leading to a Drude-like formula in which the inverses of the disorder and interaction scattering times enter in a simple additive form. We also make contact with earlier theories of the transverse spin susceptibilities and with the spin-pumping picture of the Gilbert damping.

1Work supported by NSF Grants DMR-070540 and DMR-0313681

12:27PM J32.00005 FMR Investigations on Ni-Co thin films1, JUSTIN BAIZE, The University of Texas Pan American, STEVEN MICHALSKI, ROGER D. KIRBY, University of Nebraska Lincoln, MIRCEA CHIPARA, DAVID J. SELLMYER, University of Nebraska Lincoln — Magnetic interactions between thin films of Co and Ni spaced by a conducting, non-magnetic film (Pt) are analyzed by utilizing a Bruker ELEXYS-EPR spectrometer operating in the X-band (9 GHz). Ferromagnetic resonance spectra have been recorded at room temperature in the out-of-plane configuration, for different orientation of the external applied film relative to the plane of the sample. The effect of the metallic film (Pt) thickness on the interaction between Ni and Co is investigated. For most orientations, the ferromagnetic line of such multilayers is the result of a convolution between the lines of Ni and Co films and has been fitted by a superposition of two Lorentzian lines. The outcome of the interaction between the two magnetic layers on the position and the width of ferromagnetic resonance lines is analyzed in detail.

1ESR measurements were done within the laboratory of Professor A. Rajca from the Chemistry Department of the University of Nebraska Lincoln.

12:39PM J32.00006 Determination of ferromagnetic resonance of thin films with coplanar waveguide, XIN FAN1, TAKAIRO MORIYAMA, RONG CAO, JOHN XIAO — Determination of ferromagnetic resonance of thin films with coplanar waveguide X. Fan, T. Moriyama, R. Cao, John Q. Xiao Department of Physics and Astronomy, University of Delaware, Newark Delaware 19716 USA Recently, Coplanar Waveguide (CPW) has been applied to determine Ferromagnetic Resonance (FMR) of magnetic thin film due to its simple geometry and broadband nature. Compared to the conventional method using reflection in a resonant cavity, CPW should be interpreted by the transmission line theory, taking into account of both transmission and reflection. It has been shown that FMR linewidth extracted from S-matrix after four port calibration differs from that extracted from transmission only, which neglects the impedance mismatch effect. However, the four port calibration is rather complex and tedious. In this presentation, we introduce a new method to extract FMR spectrum without performing four port calibration. We use both transmission and reflection signals, and consider the impedance mismatch, We will demonstrate the difference between these two methods are negligibly small. 1. Y. Ding, T. J. Klemmer, T. M. Crawford, J. Appl. Phys. 96, 2969, 2004 2. C. Bilzer, T. Devolder, P. Crozat. J. Appl. Phys. 101, 074505, 2007

1Member ID will be officially activated on 12/01
12:51PM J32.00007 Magnetostatic micro-resonators. ALEXANDER KOZHANOV, ZACH GRIFFITH, MARK RODWELL, JIM ALLEN, UCSB, Santa Barbara, CA, USA, DOK WON LEE, SHAN WANG, Stanford University, Stanford, CA, — AJEY JACOB, Intell, Inc., WIN COLLABORATION — Small scale magnetostatic wave devices are potentially important for on-chip filters for communication systems and more exotic gated spin wave devices. We describe experimental results that measure transmission and reflection resonances in micron size resonators coupled to coplanar waveguides. Ferromagnetic CoZrTa films were sputtered onto Si wafers covered by SiO2 and lithographically patterned into stripes and crosses of varying length and width. Magnetostatic waves were excited and detected by overlaying coupling loops patterned as shortened coplanar waveguides. Transmission and reflection S-parameters of fabricated structures were measured in the frequency range (0-50)GHz. Transmission and reflection resonances strongly dependent on the geometry of the ferromagnetic device and applied magnetic field are observed. The results are modeled as standing magneto static waves in micro-resonators. We discuss effect of biasing magnetic fields, approaches to enhanced coupling to the magnetostatic resonators, magnetostatic wave interferometers and magnetization controlled magnetostatic wave switching in junctions. This work is supported by the Nanoelectronics Research Initiative (NRI) - Western Institute of Nanoelectronics (WIN).

1:03PM J32.00008 Measurements of spin diffusion length in gold with point contact Andreev reflection spectroscopy MUHAMMAD FAIZ, RAGHAVA PANGULURI, Physics and Astronomy Department - Wayne State University, BAKLIN BALKE, SABINE WURMEHL, CLAUDIA FELSER, Johannes Gutenberg-Universitat, Germany, ANDRE PETUKHOV, Physics Department - South Dakota School of Mines and Technology, PO Box 4100, FI-02015 HUT, Finland — A family of inhomogeneous Hubbard models is shown to have multi-level spin-switching properties. The generic structure of the device is NNMMN/MMN, which defines a linear (quasi-0D) cluster, having open boundary conditions. Within the context of the Hubbard model, N refers to a nonmagnetic (U=0) atom and M is a magnetic atom having finite value of the Hubbard U. The model is solved by numerically exact diagonalization. Localized spin-switching is obtained as a function of the electron filling and is activated by application of an external magnetic field. Arbitrary numbers of nonmagnetic atoms at the edges of the chain, relative to the number of magnetic atoms in the system, lead to a range of spin-switching signals. One potential application to be demonstrated is that of a single minority spin-flip detector.

1:27PM J32.00010 Anisotropic spin exchange between electrons mediated by spin-orbit interaction SUHAS GANGADHARAIAH, JIANMIN SUN, OLEG STARYKH, University of Utah — It is well known that the exchange coupling between electrons in the presence of Rashba spin-orbit interaction (SOI) is anisotropic. In particular, due to the SOI, electron spins are not conserved during a tunneling process as a result anisotropic exchange terms of the Dzyaloshinkii-Moriya (DM) type are generated. In this talk, we re-visit and clarify the role of spin-orbit interaction in lowering the symmetry of the exchange coupling between spins. We point out that the exchange Hamiltonian, despite of its anisotropic appearance, retains spin-rotational (SU(2)) invariance to the second order in the spin-orbital coupling. We argue that spin-rotational symmetry is broken only in the fourth order in SOI coupling. To capture this, we calculate the exchange problem along the lines of the Heitler-London approach.

1:39PM J32.00011 Noise Spectrum Signature of Large Jumps in the Magnetization of a Finite System Near a Phase Transition ZHI CHEN, CLARE YU, University of California, Irvine — It is well known that a finite-size spin system can undergo thermally driven flips of the magnetization of the system as a whole. But what is an experimentally measurable signal of this? We show that the low frequency noise spectrum of the magnetization has a distinct signature of these total magnetization flips which as particularly evident just below the phase transition temperature. To see this, we studied the magnetization and energy spectra of the 2D Ising model by using Monte Carlo simulations. We find that at $T_C$ the noise power is a power law in the frequency where the power is given by the critical exponents. As the frequency decreases for a finite system just below $T_C$, the magnetization noise spectrum crosses over to $f^{-2}$. We show that this is due to large jumps in the entire magnetization. Finally at the lowest frequencies, the noise spectrum saturates at a frequency that depends on the system size. The method we used can be applied without much modification to quantify the contribution of jumps to the dynamics of other systems.

2:03PM J32.00013 The role of uncompensated spins in exchange biasing HANS J. HUG, Empa, Materials Science and Technology, Switzerland and Institute of Physics, University of Basel, Switzerland, IRIS SCHMID, PÉTER KAPPÉNBERGER, SARA ROMER, Empa, Materials Science and Technology, Switzerland — The origin of the exchange bias (EB) effect has been traced back to the existence of pinned uncompensated spins (UCS) in the antiferromagnet (AFM) or at its interface. However, the understanding of the underlying mechanism is still clouded by contradictory reports: For example, both a parallel as well as an antiparallel orientation of the UCS relative to the magnetization direction of the ferromagnet (FM) were reported for similar FM/AFM systems. Here different magnetization histories in magnetometry and high resolution magnetic force microscopy measurements are used advantageously to demonstrate the co-existence of pinned UCS that are parallel and antiparallel to the cooling field in metallic (IrMn) and oxidic (CoO) EB systems. We further conclude that the EB effect is mainly a result of pinned interfacial UCS, which are antiparallel to the FM spins. In further experiments, the distribution of density of the UCS were imaged on the length scales of single grains. A surprisingly strong fluctuation of the local UCS density (UCSD) was observed. A correlation between the UCSD and the local exchange field was performed. Clearly, a high UCSD results in a low local exchange bias field. Regions with an anti-ferromagnetic effect were found. Using grain-boundary engineering, exchange-biased materials without such regions could be fabricated that showed a substantially increased exchange bias effect.

1 Work supported by DOE grant DE-FG02-04ER46107

11:15AM J33.00001 Ferromagnetism in Mn-implanted Ge and epitaxial GeC\(^x\). SAMARESH GUCHARIT, JOHN MARKERT, Department of Physics, The University of Texas at Austin, MUSTFA JAMIL, SANJAY BANERJEE, Department of ECE, The University of Texas at Austin — 20 keV energy Mn ions were implanted in two samples: 1) bulk Ge (100) and 2) a 250 nm thick epitaxial GeC film, grown on a Si (100) wafer. The GeC thin film was grown by UHV chemical vapor deposition using a mixture of germane (GeH\(_3\)) and methylgermane (CH\(_3\)GeH\(_3\)) gases and contains less than 1% carbon. X-ray diffraction data shows a single crystal phase for the GeC film, and the surface rms roughness is about 0.3 nm, measured with AFM. The Mn implant dose was 1.1 \times 10^{10}/cm\(^2\) at a temperature of 300°C for both samples. For this relatively low energy Mn ion implant, the range is about 17 nm and the straggles is about 9 nm. A SQUID magnetometer study shows ferromagnetism in both samples. While the Curie temperature for both samples is about 180 K, the in-plane saturated magnetic moment per unit area for the first sample is about 2.2 \times 10^{-5}emu/cm\(^2\) and that for the second sample is about 3.0 \times 10^{-5}emu/cm\(^2\). These results show clear enhancement of magnetic properties of the Mn-implanted GeC thin film over the identically implanted Ge layer due to the presence of a small amount of carbon.

\(1\)This work was supported by SWAN and NSF DMR 0605828.

11:27AM J33.00002 Influence of carrier type on the ferromagnetism in Ge\(_{1−x}\)Mn\(_x\) thin films. WENNING YIN, JIWEN LU, LI HE, JIAN YU, WENSIN FAN, ROBERT HÜLL, STUART WOLF, University of Virginia — We have been studying the magnetic and transport properties of Mn-doped Group IV semiconductors. Mn ions have been implanted into both boron doped P-type and phosphorus doped N type Ge thin films respectively. A ferromagnetic hysteresis loop has been observed in P-type samples at low temperatures and supermagnetism remains strong at 300 K. The P-type samples show much stronger ferromagnetism than N-type samples. At 5K, the ferromagnetic saturation moment (Ms) of 5% Mn-doped p-Ge sample is ~0.65 Bohr magneton per Mn, which is almost twice as much as that of the 5% Mn-doped n-Ge. Rapid thermal annealing has been used to reduce the ion implantation damage as well as to help Mn ions to incorporate into Ge lattice. In this talk we will present magnetic, transport and electron microscopy characterization of these samples. We are in the process of trying to understand the nature of the ferromagnetism in these films and its correlation to carrier type.

11:39AM J33.00003 Epitaxial Growth and Properties of Multilayers Containing (CoMn)\(_0.9\)Ge\(_0.9\) and Ge (001). LIANG HE, CHARLES MALMBERG, BRIAN COLLINS, FRANK TSUI, University of North Carolina at Chapel Hill — Epitaxial growth and magnetic and magnetotransport properties of superlattices containing Co and Mn codoped Ge magnetic semiconductor layers with Ge (001) interlayers have been studied. Layer-by-layer epitaxial growth has been observed during the deposition of the dopant magnetic semiconductor layers, i.e. (CoMn)\(_0.9\)Ge\(_0.9\), and that of the undoped Ge interlayers, as indicated by persistent oscillations in the intensity and width of reflection high energy electron diffraction. The superlattices exhibit a ferromagnetic transition near 100 K and superparamagnetism at higher temperatures, as determined by temperature and field dependent magnetic measurements using SQUID magnetometry. Magnetotransport properties indicate that the superlattices are p-type semiconductors with very large positive magnetoresistance (MR) and anomalous Hall effect (AHE). Conduction at low temperatures (\(< 100\) K) is dominated by variable range hopping in the impurity band. Below 100 K, the MR is found to scale with square of the magnetization, whereas the AHE exhibits a linear dependence on magnetization. Above 100 K, in the superparamagnetic regime the magnetotransport parameters scale with magnetic field.

1DOE DE-FG02-05ER46216 and NSF DMR-0441218

11:51AM J33.00004 Different magnetic moment in Mn-doped amorphous group-IV semiconductors: a comparison study between Si and Ge matrices. LI ZENG, ERIK HELGREN, University of California, Berkeley, CINTHIA PIAMONTEZE, ELKE ARENHOLZ, ALS, Lawrence Berkeley Lab, Berkeley, CA, ADDISON HUEGEL, FRANCES HELLMAN, University of California, Berkeley — Mn-doped amorphous Si (\(\alpha\)-Si) and Ge (\(\alpha\)-Ge) are prepared by \(\gamma\)-beam co-evaporation for a wide range of concentrations (0.5–18 at.\%) to explore the Mn local moment in group-IV semiconductors. We find that Mn behaves quite differently in these two matrices: in \(\alpha\)-Si, the Mn local moment is quenched, even for the lowest doping (0.5 at.%), while in \(\alpha\)-Ge, a large Mn moment is observed, with a spin-glass ground state. X-ray absorption spectra (XAS) of \(\alpha\)-Mn\(_{2}\)Si\(_{1−2}\) have very broad L-edge absorption peaks which correlate with the quenched magnetic state. The quenched Mn moment in \(\alpha\)-Si is unexpected and can be understood by the formation of Anderson-localized itinerant states even on the insulating side of the metal-insulator transition. (\(\alpha\)-Si, \(\alpha\)-Ge) show atomic multiplicities. \(\alpha\)-Mn\(_{2}\)Si\(_{1−2}\) has positive magnetoresistance (MR) like typical non-magnetic doped systems, while \(\alpha\)-Mn\(_{2}\)Ge\(_{1−2}\) has negative MR, consistent with magnetization data.

\(1\)This research was supported by NSF DMR-0505524.

12:03PM J33.00005 Magnetic Properties of Ge\(_{1−x}\)Mn\(_x\)Te Thin Films. JAMES R. ANDERSON, Dept. of Physics & Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD, W. KNOFF, MALGORZATA GORSKA, T. STORY, Institute of Physics, PAN, Al. Lotnikow 32/46, Warsaw, Poland, COSTEL R. ROTUNDU, Dept. of Physics & Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD — We have measured the magnetization of Ge\(_{1−x}\)Mn\(_x\)Te thin films with 0.08 < x < 0.19 at magnetic fields up to 7 T at temperatures from 2 to 385 K. The monocrystalline epitaxial layers of Ge\(_{1−x}\)Mn\(_x\)Te were grown on (111)-oriented BaF\(_2\) crystalline substrates in a home-built MBE system. The layer structure was rhombohedral, thickness in the range 0.5 – 1 micron, and hole carrier concentration of the order \(10^{21}\) cm\(^{-3}\). Magnetization measurements were made using a Quantum Design MPMS system. At low temperatures the samples were ferromagnetic. The ferromagnetic – paramagnetic transition was observed in various samples in a broad temperature range from 20 – 100 K. In some samples we have seen two peaks in the temperature dependence of the low-field magnetization. These peaks may be evident of two chemical phases or of an electronic phase separation. The origin of this effect is under investigation at the present time.

1Partial funding by CNAM.
12:15PM J33.00006 Spin Engineering with Ion Implantation of Diamond Nitrogen-Vacancy Centers¹, G.D. FUCHS, F.J. HEREMANS, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation-University of California, Santa Barbara, CA, R. HANSON, Kavli Institute of Nanoscience - Delft Institute of Technology, A. BATRA, T. SCHENKEL, Lawrence Berkeley National Lab, S. SHIRVASTAVA, T. MUGATO, E. SIDERAS-HADDAD, University of Witwatersrand, Johannesburg, S. Africa — Nitrogen-vacancy (NV) defect centers in diamond exhibit long coherence times of spin states at room temperature. Individual NV centers can be optically initialized and read-out, making them attractive candidates for quantum information. By exploiting the interactions with naturally occurring, nearby spins, NV centers have been incorporated into two quantum bit (qubit) systems. Despite these successes, scaling NV qubit systems with naturally occurring spins is a challenge. Here we present an alternative approach where we deliberately place NV centers using spatial and energy selective ion-implantation of nitrogen into synthetic diamond samples with low nitrogen content. Since we use isotopically pure N-15 for implantation, we can distinguish the implanted NV centers from the naturally occurring N-14 centers by measuring the hyperfine splitting of the electron spin resonance peaks of individual NV centers.

¹Work supported by AFOSR, FCRP, and CNID.

12:27PM J33.00007 Electronic transport in nitrogen-rich diamond¹ , F.J. HEREMANS, G.D. FUCHS, C.F. WANG, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA, R. HANSON, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — Electronic transport in carbon-based materials, including carbon nanotubes, graphene, and diamond, have been receiving significant attention as potential alternatives to silicon-based electronics. In particular, diamond’s excellent thermal properties provide a promising alternative in power-sensitive applications. Here we present studies of the photo-excited electronic transport in nitrogen-rich type IB diamonds. In addition to the study of the carrier dynamics within this system, we discuss a charge storage effect that may find potential application in charging-based memories. We find that the discharge curves follow a “stretched-exponential” form [1] with a fixed exponent, which does not depend on electrode spacing, voltage, and illumination intensity. These findings are discussed in the context of a transport mechanism in this nitrogen-rich diamond substrate.

¹This work was supported by AFOSR, FCRP, and CNID.

12:39PM J33.00008 Polarization-selective excitation of nitrogen vacancy centers in diamond . T. P. MAYER ALEGRE, Laboratorio Nacional de Luz Sincrotron, C. SANTORI, Hewlett-Packard Laboratories, G. MEDEIROS-RIBEIRO, Laboratorio Nacional de Luz Sincrotron, R. G. BEAUSOLEIL, Hewlett-Packard Laboratories — The nitrogen-vacancy (N-V) center in diamond is promising as an electron spin qubit due to its long-lived coherence and optical addressability. Nevertheless, some work remains in determining the detailed energy level structure. In particular, little emphasis has been put on the microwave polarization selection rules. In typical optically-detected magnetic resonance (ODMR) experiments, the microwave transitions are driven by linearly polarized fields. Thus the individual transitions can be selected only by applying a constant magnetic field to lift the degeneracy. Typically the magnetic field is applied along the quantization axis of the NV center to avoid mixing of the spin states. This applied magnetic field is in principle unnecessary with circularly polarized microwave excitation. Using a resonator designed to produce circularly polarized microwaves, we have investigated the polarization selection rules of the N- V center. We first apply this technique to N-V ensembles in [100] and [111]-oriented samples. Next, we demonstrate an imaging technique, based on optical polarization dependence, that allows rapid identification of the orientations of many single N-V centers. Finally, we test the microwave polarization selection rules of individual N-V centers of known orientation.

12:51PM J33.00009 Spin transport studies in high mobility organic semiconductor, Pentacene (C_{22}H_{14})¹ , J.H. SHIM, V. KARTHIK, J.S. MOODERA, MIT, MIT TEAM — Spin transport in organic semiconductors (OSs) is currently an attractive research area because these materials in general can have long spin coherence length due to weak spin-orbit scattering and hyperfine interaction. Charge and spin transport in OSs strongly depend on the intermolecular overlap of electronic wave functions and defects in OS which can be influenced by the thin film growth conditions. Here we chose OS, pentacene (C_{22}H_{14}), which is among the most promising materials due to its high mobility. From the measured temperature dependence of the conductance in Al/Pentacene/Co thin film tunnel junctions, different transport mechanisms were observed for pentacene barriers of various thicknesses. Thin, amorphous pentacene films were deposited with and without Al_{2}O_{3} seed layer at room temperature. Significant tunnel magnetoresistance (TMR) was observed at room temperature in junctions with Co and Fe electrodes and pentacene tunnel barrier. These results will be presented and discussed. Research supported by ONR and KIST-MIT programs.

¹Supported by U.S. DOE Office of Science under Contract No. DE-AC02-06CH11357.

1:03PM J33.00010 Is there really spin transport in AlQ3 spin-valves?¹ , J. SAMUEL JIANG, J.E. PEARSON, S.D. BADER, Argonne National Laboratory — There have been reports of GMR and extremely long spin relaxation in AlQ_{3}-based spin valves. However, it has also been suggested that direct tunneling through locally-thin regions of the Alq_{3} layer could be the magnetoresistance (MR) mechanism, i.e. the reported MR may be due to artifacts rather than spin transport via the molecular levels in AlQ_{3}. We present transport measurements on AlQ_{3}-based spin valves and unipolar devices where the Alq_{3} thickness is beyond the tunneling limit. The I-V characteristic is highly asymmetric and strongly temperature-dependent, different from the behaviors of devices where GMR has been reported. The charge transport in the Co/AlQ_{3}/Fe spin valves is by holes only and is injection-limited. More importantly, we observe no measurable MR in our non-tunneling Co/AlQ_{3} /Fe spin valves, or in Co/Al_{2}O_{3}/AlQ_{3}/Fe structures where spins can be injected via the AlQ_{3} barrier. These results indicate that spin transport in AlQ_{3} is unlikely.

¹Supported by U.S. DOE Office of Science under Contract No. DE-AC02-06CH11357.

1:15PM J33.00011 Inelastic tunneling spectroscopy study on organic semiconductor tunnel barriers with magnetic electrodes¹ , K.V. RAMAN, J.H. SHIM, J.S. MOODERA, MIT — Spin injection and transport through organic semiconductor (OS) is recently being researched extensively. Exploring the interfacial structural and chemical modifications in FM/OS/FM tunnel junctions can lead to a better understanding of spin injection and transport in OS. Inelastic tunneling spectroscopy (IETS), a high sensitivity technique, measures the vibrational and excitational modes of the molecules within a tunnel barrier, which are greatly influenced by any distortions in the molecules. These measurements are performed on thin films of OS, rubrene and pentacene, using Co/seed/OS/Pt and Al/seed/OS/Al junctions, all grown in-situ, for two different seed layers viz. AlQ_{3} and LIF. The IETS spectra matches well with the reported Raman and IR spectroscopy measurements performed for powder and bulk single crystal samples. In addition, the IETS spectra show weak signatures of the molecular distortions through modification of certain phonon peaks. Due to the amorphous nature of the films certain electronic states are also observed at higher bias voltages. The effect of vibrational modes on the spin conserved tunneling and the effect of different electrodes on the IETS spectra will also be presented and discussed.

¹Research supported by ONR and KIST-MIT programs.
1:27PM J33.00012 Spin transport studies through spin filter and organic semiconductor hybrid tunnel barriers. DEUNGJANG CHOI, Ewha University, TIFFANY SANTOS, Argonne National Lab, TAE HEE KIM, Ewha University, JAGADEESH MOODERA, Francis Bitter Magnet Lab, MIT — Spin polarized tunneling through a hybrid tunnel barrier of spin filter EuO magnetic semiconductor and an organic semiconductor Rubrene was investigated. With magnetic tunnel junction structures such as Co/Rubrene/EuO/Al or Cu we observed a magnetoresistance (MR) of up to 8.5%, whereas from the junction resistance versus temperature data, we deduced the capability to produce spin polarization (P) of up to 99%. Thus the observed low MR has been attributed to spin scattering by defects at various EuO and Rubrene interfaces and possible nonstoichiometry in EuO. With further optimization it should be possible to reach towards the expected large MR in such systems. Moreover, Rubrene which has a low barrier height also serves to magnetically decouple the ferromagnetic electrode from EuO, necessary for independent magnetic switching and reaching high MR. This study demonstrates the possibility of combining organic and spin filter materials as tunnel barriers.

1:39PM J33.00013 Quantitative analysis of molecular spintronics. ZHANYU NING, YU ZHU, JIAN WANG, HONG GUO, McGill University, HONG GUO TEAM, JIAN WANG TEAM — We report quantitative analysis of nonequilibrium spin injection from Ni contacts to octanethiol molecular spintronic system. Our calculation is based on carrying out density functional theory within the Keldysh nonequilibrium Green’s function formalism. The first principles results allow us to establish a clear physical picture on how spins are injected from the Ni contacts through the Ni-molecule linkage to the molecule, why tunnel magneto-resistance is rapidly reduced by the applied bias in an asymmetric manner, and to what extent ab initio transport theory can make quantitative comparisons to the corresponding experimental data. We found that extremely careful sampling of the two-dimensional Brillouin zone of Ni surface is crucial for accurate results.

1:51PM J33.00014 Hall conductivity and colossal magnetoresistance in FeSb2. RONGWEI HU, Condensed Matter Physics, Brookhaven National Laboratory, VESNA MITROVIC, Physics Department, Brown University, CEDOMIR PETROVIC, Condensed Matter Physics, Brookhaven National Laboratory — We report the anisotropic Hall conductivity and discuss mechanism of colossal magnetoresistance in Co doped FeSb2. The Hall conductivity is described in a multi-carrier picture, in which large carrier mobility was found in Co doped FeSb2.

2:03PM J33.00015 Electric field induced metal-insulator transition and colossal magnetoresistance in CdCr2S4. C.P. SUN, C.C. LIN, J.L. HER, S. TARAN, C.C. CHOU, C.L. CHAN, C.L. HUANG, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — Multiferroic ordering existing in a single material is a recent hot topic in the field of condensed matter physics due to its potential application in device control. The chromium chalcogenide spinel CdCr2S4 is one of the attractive materials investigated by Hemberger et al. recently. Based on the electrical measurement, there is no discontinuity through the ferromagnetic ordering at TC ∼ 85K. [2] We measure the temperature dependent resistance under various electric fields to investigate the electrical properties of the present material. To our knowledge, we first observe the electric field induced metal-insulator transition in this material around TC. Moreover, a colossal magnetoresistance (CMR), which is comparable to that of manganese-based CMR material, is also observed near TC. The origin for these properties is discussed. [1] J. Hemberger, P. Lunkenheimer, R. Fichtl, H.-A. Krug von Nidda, V. Tsurkan, A. Loidl, Nature 434, 364 (2006). [2] P. K. Baltzer, H. W. Lehmann, and M. Robbins, Phys. Rev. Lett. 15, 493 (1965).
12:03PM J35.00003 Fullerene microcrystals under pressure¹, MURILO L. TIAGO, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — Solid buckminsterfullerene ($C_{60}$) is known to be very soft, with a large number of crystalline phases that can be accessed by temperaturer or pressure. External pressure reduces the intermolecular distance, which affects the electronic structure in three ways: by increasing the overlap between molecular orbitals on neighbor molecules, by inducing additional chemical bonds between molecules, and by deforming the molecular structure. Having an exciton gap that is sensitive to pressure suggests that $C_{60}$ can be used as active element in an optical pressure gauge: a device that can detect pressure dynamically by measuring the emission from the ground state of the molecule. Spectroscopic single molecule studies provide insights into the many-body theory. We calculate the optical gap of solid $C_{60}$ and its pressure dependence. We also analyze the dependence of optical gap with deformations in the molecule. Our calculations are based on solving the Bethe-Salpeter for electron-hole excitations. The electron self-energy is calculated within the GW approximation. We use pseudopotential density-functional theory to determine the electronic structure of $C_{60}$ in its ground state.

¹Research supported by the Division of Materials Sciences and Engineering BES, U.S. DOE under grant ERKCS77.

12:15PM J35.00004 Nanowire waveguide made of extremely anisotropic metamaterials¹, Y.J. HUANG, W.T. LU, S. SRIDHAR, Department of Physics and Electronic Materials Research Institute, Northeastern University, Boston, MA 02115 — We consider wave propagation along a cylindrical fiber with anisotropic optical property. Exact solutions are obtained for all the modes. For extremely anisotropic cylinder where the transverse permittivity is positive, only transverse magnetic and hybrid modes will propagate on the waveguide. At a given frequency the waveguide support infinite number of eigenmodes. For the TM modes, there exists at most one forward wave. The rest of them are backward waves. These waveguides can be used as filter and phase shifter in integrated optical circuits.

¹This work was supported by the Air Force Research Laboratories, Hanscom (Contract # FA8718-06-0-C-0045) and the National Science Foundation (contract # PHY-0457002).

12:27PM J35.00005 Doping Poly(p-phenylene vinylene) with Phosphomolybdate through Layer-by-Layer Fabrication for Optoelectronic Applications, CHRISS NELSON, BIN WANG, Lamar University — Poly(p-phenylene vinylene) (PPV) multilayers have been prepared from its cationic precursor via the layer-by-layer deposition. The photoluminescence (PL) and film thickness of the multilayers have been measured via fluorimetry and atomic force microscopy. The PL of the multilayers has been observed that is consistent with the literature results. When phosphomolybdate PMo12 is incorporated into the multilayer structure, PL quenching is detected that is proportional to the amount of PMo12 used. The quenching is interpreted as exciton diffusion through the polymer multilayers, followed by exciton dissociation at the polymer/PMo12 interface. We show that the modeling used for calculating the PL intensities derived from inorganic semiconductors is also applicable to conjugated polymers. According to the model, an exciton diffusion length is found to be 11.5±0.4 nm.

12:39PM J35.00006 Scattering studies of stacked polymer/liquid crystal composites, SAMEET SHRIYAN, KASHMA RAI, ADAM FONTECHIO, Drexel University — In this work we investigate light scattering from stacked polymer/liquid crystal composite films on several different substrates. Effect of different substrates such as glass, PET and PMMA coated with conductive layers such as Indium-Tin-Oxide (ITO) and PEDOT:PSS conducting polymer are analyzed using scattering and wavefront measurements. Scattering of light in both transmission and reflection mode is measured as a function of angle and its effect using different substrate layers coated with different conducting layers is analyzed. Shack Hartmann wavefront sensor is used to characterize the effect of various substrate and conducting layers on the transmitted wavefront quality in both transmission and reflection mode. Optimal stack length at which the scattering and wavefront degradations are at acceptable levels is derived from the scattering and wavefront measurements. Spectrometry results show notch formations at different wavelength and the effect on transmitted baseline reduction due to scattering using different substrates. SEM imaging shows the effect of different substrates and conducting layers on the formation and quality of gratings along with the LC droplet size which contributes to scattering. Optical path and stack length reduction of up to 45% for a stack of 10 layers is confirmed.

12:51PM J35.00007 Broadband Wavelength Spanning Holographic Polymer Dispersed Liquid Crystals, KASHMA RAI, SAMEET SHRIYAN, ADAM FONTECHIO, Drexel University — Broadened interaction wavelength of holographic polymer dispersed liquid crystals (HPDLCs) have extensive applications in beam steering for instrument clusters, hyperspectral imaging, wavelength filtering and construction of lightweight optics. A novel simultaneous time and spatial multiplexing formation configuration is proposed here, to increase narrow wavelength reflecting notch to broad range wavelength spanning device. HPDLC films have electro-optic controllability by applying field. No moving parts, light weight, small footprint compared to prisms and lenses, high color purity make the broadband wavelength HPDLCs desirable for the above applications. Varying the incident laser beam exposure angles using motorized rotating stage, during formation is the key step here for their formation in a single medium. The fabricated broadband wavelength sensitive HPDLCs are characterized for the uniformity of the reflected peak and electro optic response. Their output wavelength is analyzed using wavefront analysis technique.

1:03PM J35.00008 1.54 µm emitters based on monolithic integration of Er doped GaN with nitride emitters, RAJENDRA DAHAL, CRIS UGOLINI, ASHOK SEDHAIN, JINGYU LIN, HONGXING JIANG, Kansas State University, JOHN ZAVADA, US Army Research Office, North Carolina — Er doped III-nitride semiconductors have emerged as very promising materials for applications in photonics devices due to their novel optical and physical properties. Optoelectronic and photonic devices based on Er doped GaN are expected to meet the demand for next generation telecommunication devices due to efficient and temperature stable 1.54 µm emission from Er doped GaN. We report here on the successful fabrication of a chip size current injected 1.54 µm emitters based on monolithic integration of Er doped GaN epilayers with 365 nm nitride light-emitting diodes (LEDs). Er doped GaN and In$_{0.16}$Ga$_{0.84}$N epiayers were grown on sapphire substrates by metal organic chemical vapor deposition (MOCVD). The photoluminescence excitation (PLE) and absorption spectra of these epiayers were investigated to understand the 1.54 µm emission mechanism. A strong correlation between PLE and absorption spectra near the energy bandgap of host nitride epiayers suggest that band to band absorption and subsequent energy transfer to Er ion for 1.54 µm emission is a much more effective excitation mechanism compared to the direct absorption by Er ion. The success opens the possibility for next generation IR integrated photonic devices such as emitters, detectors, and optical amplifiers.

1:15PM J35.00009 Synthesis of Metal Silicides by Low Energy Ion Implantation, PRAKASH POUDEL, LEE MITCHELL, JIANYOU LI, BRIAN GORMAN, ARUP NEOGI, BIBHUDUTTA ROUT, JEROME DUGGAN, FLOYD MCDANIEL, University of North Texas — A 59keV Osmium beam was used to implant (5x10$^{16}$ atoms/cm$^2$) into p-type-Si (100). The implantation was performed with the ion source of a National Electrostatic Corp. 3 MV Tandem accelerator. The implanted sample was annealed at 650 °C in a gas mixture that was 4% H$_2$ – 96% Ar. Measurements showed that the samples contained a mixture of continuous polycrystalline osmium disilicide and a silicide layer. Rutherford Backscattering Analysis with 1.5 MeV Alpha particles was used to monitor the precipitate formation. Photoluminescence measurements were also performed to study possible applications of silicides in light emission.
1:27PM J35.00010 Sb-doped p-type ZnO and its application on light emitting devices1. SHENG CHU, LEELAPRASANNA J. LEELA, ZHENG YANG, JAE HONG LIM, LIN LI, JIANLIN LIU — Reliable Sb-doped p-type ZnO on silicon substrate was grown by molecular beam epitaxy. The hole concentrations up to \(10^{12}/\text{cm}^3\) were achieved by tuning the Sb cell temperature. The results from XPS and photoluminescence spectrum confirmed the theoretical prediction that the Sb doping mechanism in ZnO is the formation of complex shallow acceptor \(\mathrm{Sb}_{2n}+2\mathrm{Zn}_n\), with a low ionization energy of about 150meV. Then ZnO p-n homojunction light emitting diodes (LED) were fabricated based on the p-type Sb-doped layer, and the Ga-doped n-type ZnO layer. Low specific resistivity Au/NiO and Au/Ti contacts were deposited on top of the p-type and n-type layers, respectively, and the contacts were annealed to obtain ohmic conduction. Electroluminescence measurements were performed on the devices under different temperatures and injection currents. Strong near-band edge emissions were clearly observed at room and low temperatures. The device exhibited dominant UV peak at 3.31eV over the deep level emissions at 9K, which is the result from the large build in potential in the junction and the good film quality.

1Thanks the grant from CNID through DARPA and DMEA.

2PI

1:39PM J35.00011 2.4 \(\mu\)m GaInAsSb Mesa Photodiode Detectors: Leakage Currents and Ultimate Performance , JOHN PRINEAS, JEFF YAGER, Dept. Physics and Astronomy, University of Iowa, JON OLESBERG, Optical Science and Technology Center, University of Iowa, SHAHRAHM SEYDMOHAMADI, Dept. Physics and Astronomy, University of Iowa — Short-wave infrared photodiodes play an important role in areas such as molecular sensing, thermophotovoltaics, and astronomical study of galaxy, star, and planetary formation. Here we present results and analysis of uncoated, unpassivated, GaInAsSb mesa photodiodes. We have currently achieved room temperature peak specific detectivity \(D^*\approx6\times10^{10}\) Jones, dynamic resistance of 25 \(\Omega\)-cm\(^2\), and quantum efficiency of 50%. Devices are limited primarily by sidewall leakage currents, initially due to generation-recombination, and over time due to Ohmic leakage from buildup of sidewall oxides. Based on material parameters obtained in this as well as other studies, ultimate diode performance is predicted, and compared to extended-wave InGaAs/InP and HgCdTe detectors.

1:51PM J35.00012 Optically Active Erbium with Co-dopants in Silicon , S. ABEDRABBO, A. HADDAD, K. ALBATH, Q. YOUNIS, University of Jordan, A.T. FIORY, N.M. RAVIDRA, New Jersey Institute of Technology — Erbium impurity centers in silicon with strong optical emission properties in the near-Infrared are being sought for efficient silicon-based light sources because of the inherent advantages of integrating silicon photonics with VLSI technology. This work reports investigations of adding proper co-dopants to erbium in silicon through a cost-effective combination of techniques, comprising physical vapor co-deposition, implantation doping, ion beam mixing, and thermal annealing. Processed samples are characterized optically by photoluminescence and structurally by Rutherford backscattering.

2:03PM J35.00013 Characteristics of a Cr\(^{4+}\)-doped glass-ceramic; a new material for photonic devices , L.L. ISAACS, The City College of New York and the Graduate School of The City University of New York, New York, NY 10031, A.B. BYKOV, V. PETRICEVIC, I. POPOV, M. YU. SHARONOV, J. STEINER — The compound \(1.0(\text{Cr-doped } \text{Ca}_2\text{GeO}_4)-1.0(\text{Li}_2\text{O})-0.2(\text{Al}_2\text{O}_3)-0.5(\text{Bi}_2\text{O}_3)\), on quenching from the melt and subsequent heat treatment, yields a transparent glass-ceramic. The nanocrystallites formed by the ceramming procedure are distributed homogeneously in the bulk. Differential scanning calorimetry was used to determine the glass to crystal transformation temperature, \(T_g\), and its dependence on heating rate. The activation energy for the glass to crystallite nucleation is 62kJ/mol. The calculated Avrami exponent is 1, in agreement with scanning electron microscopy observations. X-ray diffraction data indicates that the structure of the nanocrystallites is that of distorted Cunyite (\(\text{Ca}_2\text{GeO}_4\)). Electron microscopy indicates that the crystallite sizes are less than \(1\mu\)m. The growth mode of the crystallites is “needle” like. The material exhibits broadband emission between 1050 to 1600 nm, with a maximum at \(\sim1260\) nm. The spectroscopic and optical properties indicate, that this material is a promising candidate for use in microelectronics, micro lasers and as fiber optic transmission lines.

Tuesday, March 11, 2008 11:15AM - 2:03PM — Session J36 DMP: Focus Session: Materials for Photovoltaics and Photocatalysis I — Morial Convention Center 228

11:15AM J36.00001 Polycrystalline TiO\(_2\) films with silver nanoclusters for photocatalysis . FRANK WOMACK, FEI WANG, ASOKA SEKHARAN, PHILLIP SPRUNGER, RICHARD KURTZ, Department of Physics and Astronomy, Louisiana State University — Metallic Ag nanoclusters nucleate on TiO\(_2\)(110) due to weak substrate interactions and the need to minimize their surface free energy. EELS results on single crystal TiO\(_2\) have shown that those nanoclusters have a distinct plasmon resonance at 3.7 eV which can be red-shifted when incorporated within a dielectric of titania. Polycrystalline oxides consist of mostly low surface free-energy faces and nanoclusters are expected to nucleate when dosed with Ag. We will present a combined synchrotron-based photoemission, Auger, and optical spectroscopy study of polycrystalline TiO\(_2\) films functionalized with Ag. We have made thin films of TiO\(_2\) by thermal evaporation of titanium followed by oxidation at elevated temperatures. Ag was then deposited via thermal evaporation of silver, and covered with additional layers of Ti that were subsequently oxidized and characterized with photoelectron and optical spectroscopies. We will discuss these data in the context of nanocluster formation vs bandgap doping.

11:27AM J36.00002 Buried silver nanoclusters on TiO\(_2\)(110) for photocatalysis . FEI WANG, FRANK WOMACK, ASOKA SEKHARAN, Department of Physics and Astronomy, Louisiana State University, BRENDAN WASTON, PHILLIP SPRUNGER, RICHARD KURTZ, Department of Physics and Astronomy, Louisiana State University, LSU CAMD COLLABORATION — Ag nanoclusters grown on TiO\(_2\)(110) can promote photochemistry by enhancing photoabsorption via their plasmon resonances. Overcoating the Ag clusters with a thin layer of titania red-shifts the plasmon to better match the solar spectrum and protects the nanoclusters from the environment. Our STM studies show that Ag clusters \(~5nm\) across and \(2nm\) high nucleate on the TiO\(_2\)(110) surface at room temperature. Photoemission performed at the LSU CAMD synchrotron shows that the clusters interact weakly with the substrate, although there is charge transfer from surface defects to the first nanoclusters that nucleate. EELS shows that the bare clusters exhibit a plasmon resonance located at 3.8 eV. Ti overgrowth and subsequent oxidation gives rise to new losses at about 1.5eV as observed in EELS. We will discuss our work at incorporating the nanoclusters within the titania matrix in light of their potential for producing hot electron-hole pairs for surface chemistry.
11:39AM  J36.00003  Epitaxial In$_2$O$_3$ and Sn-doped In$_2$O$_3$ thin films with (100) and (111) orientation$^1$, ERIE MORALES, Tulane University, MATTHIAS BATZILL, University of South Florida, ULRIKE DIEBOLD, Tulane University — In$_2$O$_3$ and Sn-doped In$_2$O$_3$ (Indium-Tin Oxide, ITO) have optical transparency and low electrical resistivity. Relatively little is known about their atomic-scale surface properties because of challenges in preparing single crystal samples. We have grown epitaxial In$_2$O$_3$ and ITO films on Yttrium Stabilized Zirconia. The (100) surface has polar character and the (111) orientation is non-polar. Films were prepared using oxygen-plasma assisted e-beam epitaxy under UHV conditions and the growth was monitored by RHEED. In-situ characterization with XPS, ARXPS, LEED and synchrotron-based UPS was used. In$_2$O$_3$ (100) facets while ITO(100) stays with a 1x1 termination and Sn segregates to surface. In$_2$O$_3$ and ITO (111) exhibit a 1x1 termination. On both orientations valence band maximum is 2.7 eV below the Fermi level. For the ITO films resonant photoemission measurements indicate a Sn-derived band gap state.

$^1$ NSF # CHE 0715576, CHE 010908

11:51AM  J36.00004  Epitaxial growth of In2O3(100) on Y-stabilised ZrO2(100) by O-plasma assisted molecular beam epitaxy: a study by HRTEM and XPS. ANNE BOURLANGE, DAVID PAYNE, RUSSELL EGDELL, JOHN FOORD, Dept. Chemistry, University of Oxford, OX1 3TA, PETER DOBSON, Begbroke Science park, University of Oxford OX5 1PF. JOHN HUTCHISON, Dept. Materials, University of Oxford OX1 3PH — Thin films of In2O3 have been grown on Y-stabilized ZrO2(100) by radiofrequency oxygen plasma assisted molecular beam epitaxy with a substrate temperature of 650 °C. Ordered epitaxial growth was confirmed by HRTEM and selected area electron diffraction taken across the interface between the substrate and the epilayer. Excellent crystalline order was preserved up to the surface of the films. The valence band onset in the X-ray photoemission spectra of the epitaxial films was found at 2.90 eV relative to the Fermi energy. The discrepancy between this value and the widely quoted value of 3.75 eV for the bandgap will be discussed in relation to recent theoretical work [1].


12:03PM  J36.00005  Radiation-induced defect formation and reactivity of model TiO2 capping layers with MMA: a comparison with Ru$^1$, THEODORE E. MADEY, BORIS V. YAKSHINSKIY, M. NEJIB HEDHILI, Physics Dept., Rutgers University, MANISH CHANDHOK, Intel Corp. — Our goal is to provide insights into surface processes that affect the reflectivity of TiO2- and Ru-capped multilayer mirrors used in EUV lithography by 13.5 nm (92 eV) photons. EUV-generated secondary electrons from the substrates cause surface reactions that lead to mirror contamination in background vacuum. In our experiments, low-energy electron beams mimic excitations initiated by EUV radiation. Oxygen vacancies are produced at energies above 25 eV. Carbon accumulation is measured on both Ru and TiO2 surfaces during 20 eV and 100 eV electron bombardment in methyl methacrylate vapor (MMA). The initial rates on the clean surfaces are very different: a C film grows more rapidly on TiO2 than on Ru. However, the limiting growth rates are the same for C thicknesses greater than ~1 to 1.5 nm, when MMA interacts with a C film. Irradiation of the C films in O2 gas has a mitigating effect.

$^1$Supported by Intel

12:15PM  J36.00006  In-situ vacuum studies of photocatalytic oxidation of isopropanol on nanometer thick TiO2 films grown on silicon , D. KAZAZIS, Brown Univ, Providence, RI, S. GUHA$^1$, N.A. BOJARCZUK, IBM T.J. Watson Research Center, Yorktown Heights, NY, H.-C. KIM, IBM Almaden Research Center, San Jose, CA, A. ZASLAVSKY, Brown Univ, Providence, RI — We report on measurements of the photocatalytic activity of ultra-thin TiO2 films grown on n and p type Si wafers. Using the oxidation of isopropanol to acetone as a model reaction, photocatalytic studies were carried out in-situ, in a high vacuum chamber equipped with leak valves for injecting isopropanol, oxygen and water vapor onto the TiO2 sample. The sample was irradiated through a quartz window with a UV strobe light source. The reaction was monitored with a line-of-sight mass spectrometer coupled to a lock-in amplifier tuned to the strobe frequency. We find that the photocatalytic efficiency is enhanced as the TiO2 thickness is reduced from 50nm to 2nm. We also find that the efficiency is enhanced by lowering the substrate Fermi level in going from n type to p type Si. The results strongly point to the hypothesis that only near surface electron-hole pair generation is relevant to the photocatalytic process; and that the reaction rate can be controlled by varying the substrate Fermi level which in turn changes the electrostatic potential variation within the heterostucture.

$^1$to whom enquiries should be addressed

12:27PM  J36.00007  Generation of Organic Radicals During Photocatalysis on TiO2$^1$, MICHAEL HENDERSON, Pacific Northwest National Laboratory — It is well-known that water-related radicals (such as OH$^·$ species) are produced by charge transfer events at UV-irradiated TiO2 surfaces. In contrast, organic radicals are generally viewed as being formed by reactions with OH$^·$ groups and not by direct charge transfer events. Using rutile TiO2(110) as a model photocatalyst, we show that organic radicals are generated in single-step charge transfer events during photodecomposition of adsorbed carboxylates and ketones. Some organic radicals (e.g., methyl) are ejected from the surface and, in high surface area catalysts, experience reactions away from the surface of origin. Other radicals (e.g., ethyl and t-butyl) have limited ability to escape the surface of origin without capture and subsequent thermal reactions. Understanding the chemistry associated with organic radical formation on TiO2 opens the door for more detailed examinations of charge transfer dynamics and energy redistribution during photon-initiated reactions important to heterogeneous photocatalysis.

$^1$Supported by the U.S. DOE, Basic Energy Sciences, Division of Chemical Sciences.

1:03PM  J36.00008  Photocatalytic reaction of catechol on rutile titanium oxide , PETER JACOBSON, CHUNDAO WANG, ULRIKE DIEBOLD, Tulane University — In an attempt to understand the fundamental aspects of photocatalysis we have studied the substituted benzene catechol on TiO2(110). Previous studies have given detailed information about the catechol bonding configuration letting our group focus on molecular level interactions with scanning tunneling microscopy and X ray photoelectron spectroscopy. Under UV exposure (248 nm) in an oxygen background, catechol is observed to degrade via oxidation. This oxidation process results in removal of roughly 10% of the initial monolayer. The removal of carbon from the TiO2 surface is shown to depend upon the background gas. Formation of a residual carbon layer is achieved by annealing the catechol monolayer to 600°C. This carbon layer is more difficult to remove by photocatalytic oxidation than a pristine catechol monolayer. Work supported by Intel Corporation.
1:15PM J36.00009 Water on anatase TiO2(101): a scanning tunneling microscopy study . Y.B. HE, O. DULUB, L.H. YING, U. DIEBOLD, Tulane University, C. DI VALENTIN, Universita degli Studi di Milano-Bicocca, Italy, A. TILOCCA, University College London, UK, A. SELLONI, Princeton University — The discovery of photochemical water splitting on TiO2 has motivated numerous studies of water on the surfaces of this important photocatalytic material. Previous temperature-programmed desorption and X-ray photoelectron spectroscopy studies of water on anatase TiO2(101), the most stable surface of the photocatalytically efficient anatase form, have revealed that water adsorbs molecularly on the surface in accordance with theoretical predictions. In the present study, we have employed low-temperature scanning tunneling microscopy to study water adsorption on anatase TiO2(101). We dose various amounts of water (0.2-1.8 Langmuir) at sample temperature T~130 K. Besides confirming that water favors molecular adsorption, atomically resolved STM images further reveal that water molecules adsorb at Ti5c sites forming preferentially one-dimensional chains with local doubling of the periodicity along the [010] direction. Near room temperature, the water molecules become mobile and hop between the Ti5c sites. Density Functional Theory calculations are underway to clarify the origin of the observed doubling of periodicity.

1:27PM J36.00010 Chemical Deposition and Photoactivity of Anatase and Rutile TiO2 Films on Si(111) . JOHN F. ANDERSON, University of Louisiana at Monroe, ERIE MORALES, ULRIKIE DIEBOLD, Tulane University — Dilute Aqueous Chemical Bath Deposition (CBD) from highly acidic (pH < 1) TiCl3 HCI solutions at room temperature and slightly higher (23°C – 40°C) produced thin titanium dioxide films on clean Si(111). We report initial results of X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD) measurements. The films thicknesses varied from 300 nm to ~ 1μm. It was found that the films required annealing to ensure adherence to the Si(111) substrate. XRD showed that the anatase and rutile structures were present in the TiO2 as a function of post-deposition annealing temperature. Additionally, photo decomposition results of methyl orange and methyl blue on TiO2/Si(111) system under UV light is observed and reported.

1:39PM J36.00011 Photoinduced Desorption of O2 and Photooxidation of Organics from TiO2(110) Surfaces . DAVID SPORLEDER, DANIEL WILSON, Stony Brook University, MICHAEL WHITE, Brookhaven National Lab and Stony Brook University — We present here, a study of photoinduced O2 desorption from, and reaction with coadsorbates on, a single crystal rutile TiO2(110) surface. Translational energy distributions of O2 desorbed with a photon excitation energy between 3.5 and 4.2 eV were measured using a pump-probe, time-of-flight (TOF) method. This method utilized a one-photon VUV ionization scheme for product detection that was developed in our lab. The translational energy distribution was found to be trimodal, indicating that different O2 species (i.e. O2 or O2−) or binding sites may play a role. It was found that the O2 translational energy distributions did not depend on the excitation energy over the range studied, which is consistent with a substrate mediated excitation mechanism involving hole capture. More recent experiments are exploring the mechanism for photooxidation of organic molecules. Specifically, we are determining translational energy distributions of small radicals originating from photoinduced fragmentation of simple ketones on a TiO2(110) surface.

1:51PM J36.00012 Influence of the Sensitizer Protonation and Adsorption Mode on the Efficiency of Dye-sensitized solar cells . ANNABELLA SELLONI, Princeton University, FILIPPO DE ANGELIS, SIMONA FANTACCI, Universita’ di Perugia, Italy, MOAMMHD NAZERUDDIN, MICHAEL GRAETZEL, Swiss Federal Institute of Technology, Lausanne, Switzerland — Dye sensitized solar cells (DSSCs) represent a promising approach to the direct conversion of light into electrical energy at low cost and with high efficiency. In these devices, a dye sensitizer absorbs the solar radiation and transfers the photoexcited electron to a nanostructured TiO2 electrode. We have studied the electronic structure of different Ru(II)-polypyridyl dyes adsorbed onto a model TiO2 nanoparticle by means of first principles Density Functional Theory calculations. Our results suggest that two different electron injection mechanisms (adiabatic and non-adiabatic) may be present in DSSCs employing dyes carrying a different number of protons. We also found that sensitizers with inequivalent pyridine ligands exert strong dipolar fields at the TiO2 surface, causing a conduction band down-shift and a reduction of the cell open circuit potential, thus resulting in a reduced DSSC efficiency.

Tuesday, March 11, 2008 11:15AM - 2:15PM Session J37 FIAP: QHE: Bilayers and Graphene Morial Convention Center 229

11:15AM J37.00001 Thin cylinder limit of Halperin bilayer quantum Hall states . ALEXANDER SEIDEL, Washington University in St. Louis, KUN YANG, National High Magnetic Field Laboratory, Florida State University — The traditional framework to study fractional quantum Hall states is based on Laughlin type wavefunctions and Chen-Simons field theories. Recently, a new framework has been proposed that puts stronger emphasis on the one-dimensional (1d) Hilbert space structure of Landau levels. One way to obtain this framework is by observing that states describing fractional quantum Hall liquids may be adiabatically evolved into simple one-dimensional charge-density-wave (CDW) patterns when the system is deformed, e.g., into a thin torus or cylinder. Many general properties of fractional quantum Hall systems are rooted in these CDW states, such as degeneracies and phase diagrams. In this talk, the thin cylinder limit of Halperin (m,m',n) bilayer quantum Hall states will be discussed. The corresponding CDW patterns are quite complicated for general (m,m',n), and can be worked out from a discrete version of the plasma analogy in a "squeezed space". The simpler cases map onto well-known spin-1/2 physics. This has some implications for a possible phase transition of the (331) state into the Moore-Read state.

11:27AM J37.00002 Metamorphism of quantum Hall bilayer state into a composite fermion metal . B. KARMAKAR, V. PELLEGRINI, NEST and Scuola Normale Superiore, Italy, A. PINCZUK, Columbia University, NY, L.N. PFEIFFER, K.W. WEST, Bell labs, Alcatel-Lucent NJ — In the regime of strong interlayer correlation and tunneling gap ∆_{SAS}>0, the quantum Hall (QH) ground state of bilayers at filling fraction νf=1 can be viewed as an excitonic insulator [1]. Here it will be shown that a phase transition occurs between this excitonic state and a composite-fermion metal state as ∆_{SAS} decreases [2,3]. The observations are based on inelastic light scattering of spin-wave (SW) mode at the Zeeman energy and spin-flip (SF) mode across ∆_{SAS}. These experiments show that the SF mode excitation collapses to the SW and disappears at a critical value of ∆_{SAS} while a low energy continuum of spin transitions below the SW mode appear. These transitions are interpreted as spin-flip SF excitations of the CF metal in which orientation of spin and CF Landau level index change simultaneously. Measurements of SW excitations at ∆_{SAS} will be also shown [4]. The behavior of the SW thermal activation gap as a function of the Zeeman energy suggests a subtle competition between interlayer correlation and spin effects in the broken-symmetry QH state at ∆_{SAS}≈0. [1] S. Luin, et al., PRL. 94, 146804 (2005); [2] S. Luin, et al., PRL. 97, 216802 (2006); [3] B. Karmarkar, et al., Solid State Comm. 143, 504 (2007); [4] B. Karmarkar, et al., work in progress.

11:39AM J37.00003 Evidence for a finite temperature phase transition in a bilayer quantum Hall system . A.R. CHAMPAGNE, J.P. EISENSTEIN, Caltech, L.N. PFEIFFER, K.W. WEST, Bell Labs — We study the Josephson-like interlayer tunneling signature of the quantum Hall bilayer excitonic state at total filling factor νf = 1 as a function of the layer separation, interlayer charge imbalance and temperature. The tunneling amplitude collapses to zero as either the temperature or interlayer spacing is increased. The interlayer tunneling amplitude dependences on the layer spacing at various temperatures are very similar, but the layer separations where the tunneling disappears scale linearly with temperature. Our results offer evidence [1] that a finite temperature phase transition separates the interlayer coherent phase from incoherent phases which lack strong interlayer correlations. The phase boundary is found to be re-entrant as a function of charge imbalance thus suggesting an intricate competition between the interlayer coherent phase and various independent layer states. This work was supported by the NSF and the DOE. [1] A.R. Champagne, J.P. Eisenstein, L.N. Pfeiffer, K.W. West, Cond-mat/0709.0718
is associated with the degeneracy of nearly degenerate Landau levels at the Dirac point compared to the four nearly degenerate levels which occur in an isolated layer. The additional degeneracy with a phonon mediated interlayer momentum transfer mechanism. Resonances are observed when the frequency of fields smaller than 1T. In addition to an unusual overall field dependence, we have discovered a series of oscillations in the drag resistivity which are periodic with the system in the quantum Hall state. We analyze the transport properties of bilayer Hall systems at total filling factor \( \nu = 1 \) in drag geometries as a function of interlayer bias, in the limit where the drag is sufficiently strong to form a transverse quantum Hall ferromagnet. We use a bosonic Chern-Simons model to describe the drag and drive layers, in qualitative agreement with experiment. We conclude with predictions for future experiments.

1US NSF under Grant Nos. MRSEC DMR-0800854, EPS-0720651 and DMR-0740433

12:15PM J37.00006 Non-perturbative approach to the quantum Hall bilayer. MILICA MILOVANOVIC, ZLATKO PAPIC, Institute of Physics, Belgrade — We study the disordering of the superfluid phase in the quantum Hall bilayer at the filling factor one with increasing distance between the layers. We find that the possibilities for ground state wave functions that describe the superfluid at an arbitrary distance fall into two universality classes. They correspond to (1) Berezinskii-Kosterlitz-Thouless (BKT) (2D XY) model of superfluid disordering in the presence of charged impurities and (2) \( \lambda \) transition (3D XY) model in a transverse invariant quantum Hall bilayer system. The BKT type of disordering likely ends with unbinding of charged pairs of neutral fermionic vortices (in a transition reminiscent of the one reported in Champagne et al.). In the transverse invariant system the ensuing quantum phase transition proceeds via condensation of loops of elementary charged vortices - merons into a topological phase associated with the toric code model.

12:27PM J37.00007 Phonon mediated resonances in bilayer magnetodrag. GOKUL GOPALAKRISHNAN, SANGHUN AN, DONGKYUN KO, YUKO SHIROYANAGI, THOMAS GRAMILA, The Ohio State University, Physics Dept., LOREN PFEIFFER, KEN WEST, Bell Labs, Lucent Technologies — The properties of the 2-dimensional electron gas (2DEG) have been studied extensively in the integer and fractional quantum Hall regimes. Much less is understood about the 2DEG at intermediate fields, where thermal fluctuations are comparable to the size of the Landau-level spacing. We have explored the electronic bilayer system with a magnetic field of up to 1T and 1.5K in fields smaller than 1T. In addition to an unusual overall field dependence, we have discovered a series of oscillations in the drag resistivity which are periodic in 1/8, but are distinct from variations in the density of states, as seen in Shubnikov-de Haas oscillations. These novel magnetodrag oscillations are consistent with a phonon mediated interlayer momentum transfer mechanism. Resonances are observed when the frequency of 2kF phonons matches an integer multiple of the cyclotron frequency, and they are suppressed as the densities of the two layers are mismatched.

12:39PM J37.00008 Unusual quantum Hall Ferromagnetism in Bilayer Graphene. BARLAS YAFIS, University of Texas at Austin, RENE COTE, Universite de Sherbrooke, ALLAN MACDONALD, University of Texas at Austin — Bilayer graphene has eight nearly degenerate Landau levels at the Dirac point compared to the four nearly degenerate levels which occur in an isolated layer. The additional degeneracy is associated with the degeneracy of \( n = 0 \) and \( n = 1 \) orbital Landau level states in the bilayer case and adds a Landau level pseudospin degree of freedom to the spin and valley pseudospins present in the single layer case. We predict broken symmetry states which lift the associated degeneracies with a Hunds rule which orders spin first, then valley, and finally the Landau-level pseudospin. It follows that a Landau level pseudospin orders at all odd total filling factors. We find unusual collective modes which are not gapped even though the system has uniaxial anisotropy, and a \( g^{1/2} \) dispersion at small \( g \) because the divergence of the pseudospin magnetization produces charges with long-range Coulomb interactions. Because of the charge carried by these collective modes, they are dipole active. We predict unusual intra-Landau-level contributions to the cyclotron resonance signal. We will also discuss unusual properties of the Skyrmions spin-textures of these quantum Hall ferromagnets.

12:51PM J37.00009 Symmetry Broken States of Dirac Fermions in Graphene with A Partially Filled High Landau Level. HAO WANG, D.N. SHENG, Department of Physics and Astronomy, California State University Northridge, F.D.M. HALDANE, Department of Physics, Princeton University — We report on numerical study of symmetry broken states of the Dirac electrons in partially filled N=3 Landau level (LL) in graphene. At half-filling, the static density-density correlation function displays sharp peaks at nonzero wavevector. Finite-size scaling shows that the peak value grows with electron number and diverges in the thermodynamic limit, indicating an instability toward a charge density wave. A weak disorder potential plays the role of selecting a symmetry broken stripe phase as the ground state from the nearly degenerated low-energy manifold. Such a quantum phase is experimentally observable through transport measurements. Associated with the special wavefunctions of the Dirac LL, both stripe and bubble phases become possible candidates for the ground state at lower filling numbers in the N=3 LL. We have also studied the ground state evolution and quantum phase transitions of the 2D electron gas at half-filled N=1 LL under an additional repulsive three-body interaction.

1:03PM J37.00010 Midgap states and the fractional quantum Hall regime in graphene quantum dots1. IGOR ROMANOVSKY, CONSTANTINE YANNOULEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Graphene quantum dots (QDs) with zigzag edges exhibit midgap single-particle states associated with such edges. At zero magnetic field (\( B \)), these states form a manifold of degenerate states similar to the lowest Landau level that forms in semiconductor QDs at high \( B \). It has been recently suggested that the midgap-state manifold in graphene dots can support correlated many-body states similar to the rotating-electron-molecule (REM) states (also referred to as rotating Wigner crystals) at high \( B \). Here, we will report systematic exact-diagonalization calculations for N = 1 - 10 QD electrons describing the REM states in graphene QDs. We anticipate that the graphene REM states exhibit for all N a single polygonal ring of localized electrons, in contrast to the multipolygonal ring configurations known from semiconductor QDs.

1Supported by the U.S. D.O.E. (FG05-86ER-45234)
2B. Wunsch et al., arXiv:0707.2948v2
Coulomb interaction and Landau level spacing


And in the Hartree-Fock approximation, the ground state energy at half filling becomes nearly symmetric under rotations of the three-component vector (N1, N2, m), with the first two components representing the Neel order parameter orthogonal to and the third component the magnetization parallel with the external magnetic field. When the symmetry breaking effects arising from the lattice, Zeeman coupling, and higher Landau levels are included the system develops a quantum critical point at which the antiferromagnetic order disappears and the magnetization has a kink. The observed incompressible states at filling factor one are argued to arise due to a finite third component of the Neel order parameter at these electron densities. Recent experiments appear consistent with N1=N2=0, and N3 finite, at the filling factors zero and one, respectively.

The Neel order parameter at these electron densities. Recent experiments appear consistent with N1=N2=0, and N3 finite, at the filling factors zero and one, respectively.

The observed incompressible states at filling factor one are argued to arise due to a finite third component of the Neel order parameter at these electron densities. Recent experiments appear consistent with N1=N2=0, and N3 finite, at the filling factors zero and one, respectively.

### 1:27PM J37.00012 Phase Diagram for Quantum Hall States in Graphene

JIANHUI WANG, ANDREW IYENGAR, HERB FERTIG, Indiana University, LUIS BREY, CSIC-Madrid — We investigate integral and half-integral fillings (uniform and unidimensional stripe states respectively) for graphene using the Hartree-Fock approximation in the continuum limit. For fixed filling factor, the ratio between the scales of the Coulomb interaction and Landau level spacing g = (e^2/εL)/hνF is a field independent constant. However, when B decreases, the number of filled negative Landau levels increases, which surprisingly turns out to decrease the amount of Landau level mixing. The resulting states at fixed filling factor ν (for ν not too big) has very little Landau level mixing even at arbitrary weak magnetic fields. This means many different phases should emanate from the origin of the phase diagram when plotted in the B v.s. density plane, in contrast to regular 2 dimensional electron gas which has a Wigner crystal state in the vicinity of the same point. The stripe amplitudes scale roughly as B, so that the density waves "evaporate" continuously as B → 0. These results will be compared to those of tight binding calculations.

### 1:39PM J37.00013 Chirality Sum Rule in Graphene Multilayers

HONGKI MIN, ALLAN H. MACDONALD, The University of Texas at Austin — We show that the low energy electronic structure of arbitrarily stacked graphene multilayers with nearest-neighbor interlayer tunneling consists solely of chiral pseudospin doublets. Although the number of doublets in an N-layer system depends on the stacking sequence, the pseudospin chirality sum is always N. It follows that N-layer stacks always have N distinct Landau levels at E = 0 for each spin and valley, and that the quantized Hall conductivity σxy = ±(4e^2/ℏh)/N(2 + n) where n is a non-negative integer.

This work was supported by the Welch Foundation, by NSF-NRI SWAN, and by the National Science Foundation under grant DMR-0606489.

### 2:03PM J37.00015 Lattice-Induced Double-Valley Degeneracy Lifting in Graphene by a Magnetic Field

I.A. LUK'YANCHUK, University of Picardie, Amiens, 80039 France, A.M. BRATKOVSKY, Hewlett-Packard Labs, California 94304 — We show that the recently discovered double-valley splitting of the low-lying Landau level(s) in the Quantum Hall Effect in graphene can be explained as a perturbative orbital interaction of intra- and inter-valley microscopic orbital currents with a magnetic field. This effect is provided by the translationally-non-invariant terms corresponding to graphene's crystallographic honeycomb symmetry but do not exist in the relativistic theory of massless Dirac Fermions in Quantum Electrodynamics. We discuss recent data in view of these results [1]. [1] I.A. Luk'yanchuk and A.M. Bratkovsky, arXiv:0707.0466 (2007)

Tuesday, March 11, 2008 11:15AM - 2:15PM — Session J39 DMP GSNP: Focus Session: Friction and Contact Morial Convention Center 231

### 11:15AM J39.00001 A rigorous approach to the contact mechanics of rough, elastic solids

MARTIN MUSER, Univ Western Ontario — The basic ideas of a statistical field theory is presented, which allows one to calculate the displacement field and the pressure distribution P(r) in a contact formed by an elastic body and a rigid counter face of arbitrary topography. The theory is a cumulant expansion, which contains Persson’s contact mechanics theory as the leading-order term. The cumulant approach provides a framework which correction terms can now be systematically derived. Comparison is made to numerical data for surfaces that interact via exponentially repulsive forces.

### 11:27AM J39.00002 Molecular dynamics studies of contact mechanics: contact area and interfacial separation from small to full contact

CHUNYAN YANG, BO PERSSON, IFF, FZ-Juelich, D-52425, Germany — We report a molecular dynamics study of the contact between a rigid solid with a randomly rough surface and an elastic block with a flat surface. We study the contact area and the interfacial separation from small contact (low load) to full contact (high load). For small load the contact area varies linearly with the load and the interfacial separation depends logarithmically on the load [1-4]. For high load the contact area approaches to the nominal contact area (i.e., complete contact), and the interfacial separation approaches to zero. The present results may be very important for soft solids, e.g., rubber, or for very smooth surfaces, where complete contact can be reached at moderate high loads without plastic deformation of the solids.

References:

Financial support from NSERC and GM, Canada is gratefully acknowledged.
11:51AM J39.00004 Local contact stress measurements at a rough interface, JULIEN SCHEIBERT, ALEXIS PREVOST, EYTAN KATZAV, MOHKTAR ADDA-BEDIA, GEORGES DEBRÉGEAS, LPS-ENS, CNRS-UMR 8550 Paris, France — An original MEMS-based force sensing device has been designed. It allows for spatially resolved measurements of both normal and tangential stress fields at the base of an elastomeric film in contact with a rigid substrate [1]. Model contact geometries involving a rough, nominally flat film pressed against smooth spherical and cylindrical glass substrates have been studied. In two different regimes, normal indentation and steady sliding. The measured stress profiles have been compared to calculations which assume a smooth contact obeying Amontons-Coulomb’s friction law. For the normal indentation a Finite Elements method was used, whereas for the sliding regime a semi-analytical model was developed. These direct comparisons showed that our device was accurate enough to discriminate between dry and lubricated contact conditions and evidenced load-dependent deviations from Amontons-Coulomb’s profiles. These deviations are qualitatively interpreted by taking into account the finite compliance of the contacting micro-asperities population. [1] J. Scheibert et al., arXiv:0711.117v1

12:03PM J39.00005 Friction induced displacement and stress fields within contacts with elastomers, ANTOINE CHATEAUMINOIS, CHRISTIAN FREIGNY, ESPCI, ESPCI TEAM — Friction is known to be associated with strongly heterogeneous stress and displacement fields within the contact zone. However, experimental approaches are often based on the measurement of friction forces (or mean shear stress), which makes difficult a detailed analysis of interface dynamics within sliding contacts. We have developed a new methodology for the determination of the interface shear stress distribution within macroscopic sliding contacts. It is based on an in situ measurement of the displacement field induced at the surface of highly deformable solids such as elastomers. An inversion of this field using contact mechanics models then provides the interface shear stress distribution. The experiments were carried out using two different contact configurations. The first one involves the linear sliding of a glass sphere on the elastomer substrate. The second one corresponds to an original torsional contact configuration which minimizes bulk viscoelastic dissipation during steady state sliding. Experimental distributions of frictional shear stress will be discussed in the light of theoretical models assuming either a constant interface shear stress (Tabor’s model) or a local Coulomb’s friction law.

12:15PM J39.00006 Optical measurements of pressure and displacement fields at a rough interface, ALEXIS PREVOST, JULIEN SCHEIBERT, GEORGES DEBRÉGEAS, LPS-ENS, CNRS-UMR 8550 Paris, France — We report on optical measurements of both pressure and displacement fields at the interface between a rough, nominally flat transparent elastomeric film and a smooth spherical glass lens. The multi-contact interface is imaged by transmission and the pressure field is deduced from the spatial distribution of the transmitted light. The displacement field is measured using Digital Image Correlation, focusing on a macroscopic scale. For normal loading, the mean surface pressure is measured using Hertz theory, as expected for a rough interface. A good quantitative agreement has been obtained within the statistical description of a rough sphere-on-plane contact by Greenwood and Tripp. When the interface is tangentially loaded below the macroscopic sliding threshold, analysis of the displacement field has shown a coexistence between an inner stuck region and an outer slipping annulus, as suggested by Catteneo and Mindlin. Quantitative comparison with this model yields a good overall agreement. However, small deviations are observed and can be related to the tangential compliance of the rough layer.

12:27PM J39.00007 Beller Lectureship Talk: Crack-like processes govern the onset of frictional motion, JAY FINEBERG, The Hebrew University — The dynamics of frictional slip have been studied for hundreds of years, yet many aspects of these everyday processes are not understood. One such aspect is the onset of slip. First described by Coulomb and Amontons as the transition from static to dynamic friction, the onset of frictional slip is central to fields as diverse as physics, tribology, the mechanics of earthquakes and fracture. We study the dynamics of how this transition takes place by performing real-time visualization of the true contact area which forms the interface separating two blocks of like material. The results show that the onset of frictional motion is driven by the interplay of three different types of coherent crack-like fronts, which propagate along the interface, reducing the contact area as they progress. Two of these, whose propagation speeds are, respectively, slightly below and significantly above the shear wave velocity, appear to be related to known propagation modes of shear cracks. The third type of front does not correspond to known fracture modes. It propagates over an order of magnitude more slowly, and is the most efficient of the three modes in reducing contact area along the interface. We first show that, at applied stresses that are well below the (Coulomb-Amontons) threshold for the onset of frictional motion, significant precursor activity occurs along the interface. This activity is comprised of propagating (subsonic) shear cracks which arrest before traversing the entire interface. In their wake, these “precursor” cracks systematically transform the initial spatially uniform contact area along the interface to a highly nonuniform one. Only at the transition to overall motion will these precursor cracks simultaneously excite, at their point of arrest, both the slow propagation modes and the intersonic ones. Until to this point, no overall frictional motion occurs. Frictional sliding only takes place when either the slow modes or additional shear cracks excited by the slow modes traverse the entire interface. These results suggest that to understand the transition to frictional motion, the dynamics of this entire chain of events must be taken into account.

1:03PM J39.00008 Precursor events and the onset of frictional sliding, ANDRÁS LIBAL, MARK ROBBINS, Johns Hopkins University — The precursor events leading to steady state sliding friction are investigated using a simple two-dimensional model of a rectangular block on a flat surface. As in experiments[1], a succession of cracks nucleates from the rear of the block. Each propagates rapidly and then arrests after a distance that scales with the height at which the lateral force is applied to the block. The propagation distance grows with each successive crack until a steady sliding state is attained. The distributions of local shear stress at the interface can be obtained directly in our simulations. The relation between this stress distribution, the static friction, the normal load, and the nucleation and propagation of successive cracks will be discussed. [1] S.M. Rubinstein, G. Cohen and J. Fineberg, PRL 98, 226103 (2007)
and we predict a melting temperature of about 6500 K at the core-mantle boundary. We will also present results on simulating the melting temperature of the GGA. Those systems which were too hot melted within 10 ps. Those which didn't remained with both solid and melt coexisting in the super-cell for over 25 ps.

We used 900 atoms (a 3x3x5 super-cell) with atoms in one half of the super-cell melted and the other half solid. Both halves are thermalised to the desired temperature, therefore, ab initio molecular dynamics simulations to predict its melting temperature throughout the Earth's mantle using the coexistence method. things as the crystallisation of the Earth's mantle from a magma ocean or the existence of melt in the current mantle, the melting temperature of the lower

lattice, as well as influences of the tip shape.

sliding: While some particles show finite friction increasing linearly with interface area, thus reinforcing Amontons’ law at the nanoscale, other particles assume a state of frictionless or ‘superlubric’ sliding. Additional experiments revealed a similar result even in air, which can be explained by contamination effects of the interface that alter the frictional properties.

Dragging shadows causes real friction: sliding Moiré’ patterns. A. VANOSSI, CNR-INFM S3 and Physics Dept., Modena National Laboratory, Italy, C. NEGRIT, N. MANINI, Physics Dept. and CNR-INFM, Milan University, Italy; SSISA and INFM-CNRR Democritos, Trieste, Italy, G.E. SANTORO, E. TOSATTI, SSISA, INFM-CNRR Democritos, and ICTP, Trieste, Italy — Surface Moire’ patterns are shadow-like modulations (kinks) which form at crystalline overlayers that are out of registry with their substrates. They were hardly considered in the context of friction so far, we here argue that they can be relevant. 1D model calculations suggest in fact that under the action of an external slider, the kinks are the real objects being rigidly dragged, as opposed to the real particles, which are not [1]. For a crystalline periodic slider, we predict peculiar phenomena on the fly caused by the pinning/depinning of the kink lattice to the slider, in full analogy with the well known real lattice static counterpart [2]. The frictional dissipation by a vibrating and/or sliding AFM probe should moreover be enhanced at the kinks, where atoms take poorly stable positions. Thus, AFM frictional maps [3] should reveal with much more contrast the Moire’ patterns than topographic maps of the same patterns. This concept is demonstrated by means of a simple model, which also provides a guide to the key parameters determining the enhancement. [1] A. Vanossi et al., PRL 97, 056101 (2006). [2] A. Vanossi et al., PRL 99, 206101 (2007). [3] C. Loppacher et al., PRB 62, 13674 (2000).

Contribution of Plowing to Nanotribology of Self-Assembled Monolayers. MICHAEL CHANDROSS, Sandia National Laboratories, CHRISTIAN LORENZ, King’s College, London, GARY GREST, Sandia National Laboratories, ERIN FLATER, Luther College, ROBERT CARPICK, University of Pennsylvania — Atomic force microscopy experiments and molecular dynamics (MD) simulations on self-assembled monolayer (SAM) systems have demonstrated that the nanotribology of these systems is dominated by a microscopic plowing mechanism. Due to relatively weak chain-to-chain interactions, compression only affects molecules directly under the probe tip, and not those outside the contact area. Under shear, the tip must plow into the molecules in front leading to frictional energy dissipation. We will present the results of coupled experiments and MD simulations of alkylsilane SAMs studying the plowing mechanism in detail. In particular, combinations of uncoated and SAM-coated substrates and tips are studied to probe the relationships between friction force and both contact area and applied load. As a SAM coating on the substrate (tip) is (is not) expected to result in plowing during shear, the contrast in these results, combined with detailed calculations using the MD results, will shed light on the complicated response of these systems. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

Accelerated Molecular Dynamics Simulation of AFM Experiments Using the Bond-Boost Method. WOO KYUN KIM, MICHAEL FALK, University of Michigan — We apply an accelerated molecular dynamics (MD) methodology to simulate the friction between a silicon tip and a silicon surface under perfect vacuum conditions. These simulations model recent Atomic Force Microscope (AFM) experiments which observed stick-slip motion and a lateral force showing dependence on temperature and sliding velocity. Our AFM models consist of crystalline silicon with an oxidized layer. We achieved the decrease in the simulated sliding velocity by several orders of magnitude compared with conventional MD simulations using the bond-boost method. This method is based on Voter’s hyper molecular dynamics scheme accelerating the process between slip events. The decrease in the sliding velocity makes it possible to simulate systems closer to the regime of the actual experiments. We compare the simulation results with the experimental data to elucidate the atomic level processes during sliding. We studied the effects of atomic mass transfer between the tip and the substrate on friction. Moreover, the dependence of friction on temperature and sliding velocity has been quantified, and compared with the modified Tomlinson model.

Measurement of lateral tip-sample forces in the attractive regime with picometer resolution in three dimensions. B.J. ALBERS, T.C. SCHWENDEMANN, M.Z. BAYKARA, N. PILLET, U.D. SCHWARZ, Department of Mechanical Engineering, Yale University, New Haven — Three-dimensional (3D) dynamic force spectroscopy, i.e., the acquisition of frequency shift vs. distance curves in a dense raster over a surface in order to recover the true tip-sample interaction forces with high local resolution, has so far suffered from relatively low resolution, as long-term drift stability has been a problem. Nevertheless, its promise to deliver not only the normal forces with atomic resolution, but also the lateral forces as well as the energy dissipated during an individual oscillation cycle makes it interesting for high-resolution nanotribology. Using our recently completed home-built low temperature, ultrahigh vacuum NC-AFM, we were able to map the full 3D force field over highly oriented pyrolytic graphite, which was chosen due to its qualities as a solid lubricant. Lateral forces have been measured quantitatively in a grid with spacing better than 6 pm in all three directions and pN resolution. We will discuss the distance-dependence of the static lateral forces, their local distributions with regard to the underlying lattice, as well as influences of the tip shape.

The melting curve of MgSiO3 perovskite from ab initio molecular dynamics using the coexistence method. JOHN BRODHOLT, Dept. of Earth Sciences, UCL — Despite its importance in understanding such things as the crystallisation of the Earth’s mantle from a magma ocean or the existence of melt in the current mantle, the melting temperature of the lower mantle phase MgSiO3 is poorly known. Estimates of its melting temperature at the core-mantle-boundary range from 5400 K to over 8000 K. We have used, therefore, ab initio molecular dynamics simulations to predict its melting temperature throughout the Earth’s mantle using the coexistence method. We used 900 atoms (a 3x3x5 super-cell) with atoms in one half of the super-cell melted and the other half solid. Both halves are thermalised to the desired temperature individually. We then turned off the thermalisation and allowed the system to evolve in an NV simulation, using DFT forces calculated within the GGA. Those systems which were too hot melted within 10 ps. Those which didn’t remained with both solid and melt coexisting in the super-cell for over 25 ps. These were plowed to either be on the melting curve of just below it. Our results agree well with the higher temperature melting curves found experimentally, and we predict a melting temperature of about 6500 K at the core-mantle boundary. We will also present results on simulating the melting temperature of the MgO-MgSiO3 binary.
11:51 AM J40.00002 First-Principles Molecular Dynamics of Melts in the MgO-SiO₂ System

BIJAYA KARKI, Louisiana State University, NICO DE KOKER, University of Michigan, D. BHATTARAI, Louisiana State University, LARS STIXRUDE, University of Michigan, DE KOKER COLLABORATION, STIXRUDE COLLABORATION — We have recently completed simulations of five melt compositions in the MgO-SiO₂ system within density functional theory. These results allow us to investigate the structural and thermodynamical, transport properties of melts along the MgO-SiO₂ join as a function of pressure. In particular, we have found that the mixing in MgO-SiO₂ system is significantly non-ideal at low pressures with negative excess volume and enthalpy of mixing. With increasing pressure, the volume of mixing decreases rapidly to a value close to zero at pressures above 50 GPa whereas the enthalpy of mixing remains negative. The radial distribution functions and coordination environments are found to show interesting changes with varying composition. Also, the effects of composition on diffusivity are shown to be substantial at low pressures whereas the effects are increasingly suppressed with increasing pressure.

2EAR-0409074, EAR-048182.
3Now at University College London

12:03PM J40.00003 A New look into the spin transition in Fe₂O₃

DIPTA BHANU GHOSH, STEFANO DE GIRONCOLI, SISSA and DEMOCRITOS — The wide range of intriguing characteristics exhibited by Fe₂O₃ with pressure and temperature has renewed the attention of the scientific community in the last decade. Experimental and theoretical efforts are on to address and unravel the complexity of the system. The ambient pressure phase, hematite (α-Fe₂O₃), transforms to a new structure phase (HP1). That the HP1 phase is orthorhombic perovskite (Pbnm) or Rh₂O₃-II type (Pbcm) is still a debate and yet to be explored theoretically. On top of this ambiguous assignment of HP1, there has been a long-standing issue of an isostructural high spin (HS) to low spin (LS) transition. Experimental data till date are divided into two horizons—one assigning the spin transition in the hematite phase and the other in the HP1 phase. In this work, motivated by these exotic unresolved controversies of the system, we have tried to gain an insight of the system from first principles density functional calculations. Our results favor the Rh₂O₃-II type as the HP1 phase, in agreement with recent experiments. Also a (new) mechanism governing the HS to LS transition is proposed. This mechanism, we believe, might help in removing the boundary between the two horizons as mentioned above.

12:15PM J40.00004 Prediction of an ultrahigh-pressure form of Al₂O₃

KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota — We predict by first principles a pressure induced phase transition in alumina at ~3.7 Mbar, relevant for interiors of the giant planets and terrestrial exoplanets, at room temperature from the Ca₃Al₂O₆-type polymorph to another with the U₃Si₂-type structure. This transformation should be important for the analysis of shock data in this pressure range, since alumina is used as window material. Our calculated compression curves agree with shock data excellently, indicating that the presence of two phase transitions (corundum–Rh₂O₃-II type and Rh₂O₃-II type–Ca₃Al₂O₆ type) had gone unnoticed in shock data. Our prediction suggests that the multi-Mbar crystal chemistry of planet-forming minerals might be related to that of the rare-earth sulfides.

1Research supported by NSF/EAR 0230319, 0635990 and NSF/ITR 0426757 (VLab). Computations were performed at the Minnesota Supercomputing Institute.

12:27PM J40.00005 Models of Giant Planet Interiors Derived from First-Principles Simulation

BURKHARD MILITZER, UC Berkeley, JAN VORBERGER, University of Warwick, WILLIAM HUBBARD, University of Arizona — Our understanding of the interior of giant planets is based on the accurate characterization of hydrogen and helium at megabar pressures and temperatures of several thousands of Kelvin. Theoretical methods including first principles computer simulations have been the principal tool to predict high-pressure dense fluids because laboratory experiments cannot yet probe deep into Jupiter’s interior despite great progress in shock wave measurements with precompressed samples. Results from an extensive set of density-functional molecular dynamics simulations will be presented [J. Vorberger et al., “Hydrogen-Helium Mixtures in the Interiors of Giant Planets,” Phys. Rev. B 75 (2006) 024206]. A new and more accurate equation of state (EOS) will be derived that spans the interior of giant planets. Differences from the widely used Saumon-Chabrier-Van Horn (SCVH) EOS will be analyzed. An updated model for the interior of Jupiter will be introduced. Estimates for the heavy element enrichment as well as for the size of Jupiter’s core will be discussed and compared with previous models based on the SCVH EOS. This work is supported by NASA grants PGG04-0000-0116 and NAGS-13775 as well as NSF grant 0507321.

12:39PM J40.00006 Titan’s Interior Chemical Composition: Possible Important Phase Transitions

MICHAEL HOWARD, Lawrence Livermore National Laboratory, JOSEPH ZAUG, BISHUN KHARE, CHRISTOPHER MCKAY, NASA Ames — We study the interior composition of Titan using thermal chemical equilibrium calculations that are valid to high pressures and temperatures. The equations of state are based on exponential-6 fluid theory and have been validated against experimental data up to a few Mbars in pressure and approximately 20000K in temperature. In addition to CHNO molecules, we account for multi-phases of carbon, water and a variety of metals such as Al and Fe, and their oxides. With these fluid equations of state, chemical equilibrium is calculated for a set of product species. As the temperature and pressure evolves for increasing depth in the interior, the chemical equilibrium shifts. We assume that Titan is initially composed of comet material, which we assume to be solar, except for hydrogen, which we take to be depleted by a factor 1/1000. We find that a significant amount of nitrogen is in the form of N₂, rather than NH₃. Moreover, above 12 kbars, as is the interior pressure of Titan, a significant amount of the carbon is in the form of graphite, rather than CO₂ and CH₄. We discuss the implications of these results for understanding the atmospheric and surface composition of Titan.

1Prepared by LLNL under Contract DE-AC52-07NA27344.

12:51PM J40.00007 Extended-Solid Phases of Carbon Dioxide at High Pressures

VALENTIN IOTA, ZSOLT JENEI, JAE-HYUN KLEPEIS, Lawrence Livermore National Laboratory, CHOONG-SHIK YOO, Washington State University, Pullman, WILLIAM EVANS, Lawrence Livermore National Laboratory — At high pressures and temperatures, CO₂ transforms to a series of solid polymorphs with differing crystal structures, intermolecular interactions and chemical bonding. Among them are a number of covalent (extended) solid phases, with crystal structures analogous to SiO₂ polymorphs. Above 40GPa and 1500K CO₂ transforms to phase V, a network of corner sharing CO₂ tetrahedra — structurally similar to SiO₂ tridymite. At room temperatures, CO₂ forms a-carbonia, an amorphous extended-solid phase similar to silica glass. Recently, we reported another phase, with a structure resembling that of SiO₂ stishovite, formed by compressing associated phase II above 50GPa. Here, we present a systematic picture of the structural and bonding diagram of carbon dioxide, focusing on the relationship between its molecular and extended phases at high pressures and temperatures.

1This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
1:03PM J40.00008 High-pressure Neutron Powder Diffraction and Inelastic Neutron Scattering Studies on the Mineral Jarosite KFe$_3$(SO$_4$)$_2$(OH)$_6$. MONIKA HARTL, ALICE ACATRINEI, LUKE DAEMEN, HONGWU XU, Los Alamos National Laboratory, KIM TAIT, Royal Ontario Museum, YUEJIAN WANG, SVEN VOGEL, JIANZHONG ZHANG, YUSHENG ZHAO, Los Alamos National Laboratory — The mineral jarosite KFe$_3$(SO$_4$)$_2$(OH)$_6$ has been detected in rocks at the Meridiani Planum region of Mars [1 and cited therein]. Jarosite is typically formed in aqueous environments at acidic pH. It decomposes to ferric oxhydroxides in humid climate. This gives rise to the question under which conditions jarosite was formed on Mars and what it can tell us about the climatic cycles and the former presence of water on Mars. We are looking at the phases of jarosite at elevated temperature and pressure and were able to show the stability of jarosite up to 6 GPa at room temperature and up to 3 GPa at 300 °C using neutron powder diffraction. Furthermore, we used inelastic incoherent neutron scattering to look at the vibrational modes of the hydroxyl groups in jarosite at various temperatures between 10K and 200K. [1] A. Banin, Science 309 (2005) 888

1:15PM J40.00009 Lattice Dynamics and Thermal Equation of State of Platinum. TAO SUN, Dept. of Physics and Astronomy, Stony Brook University, KOICHIRO UMEMOTO, ZHONGQING WU, Dept. of Chemical Engineering and Materials Science, University of Minnesota, JINCHENG ZHENG, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, RENATA WENTZCOVITCH, Dept. of Chemical Engineering and Materials Science, University of Minnesota — Platinum is widely used as a pressure calibration standard. However, the established thermal EOS has uncertainties, especially in the high P-T range. We use density functional theory to calculate the thermal equation of state of platinum, up to 550 GPa and 50,000 K. The static lattice energy is computed by using the LAPW method, with LDA, PBE, and the recently proposed WC functional. The electronic thermal free energy is evaluated using the Mermin functional. The vibrational part is computed within the quasi-harmonic approximation using density functional perturbation theory and pseudopotentials. Special attention is paid to the influence of the electronic temperature to the phonon frequencies. We find that in overall LDA results agree best with the experimental ones. To provide accurate thermal EOS for pressure calibration, we combine the computed temperature dependence of the Gibbs energy with the room temperature Gibbs free energy corrected by experiments. The resulting thermal EOS seems reasonably accurate and can be used as a reference for pressure calibration.

1:27PM J40.00010 Ultrafast shock wave propagation at high ambient pressure in a diamond anvil cell. MICHAEL ARMSTRONG, Lawrence Livermore National Lab, JONATHAN CROWHURST, JOSEPH ZAUG, WILLIAM HOWARD — The measurement and characterization of acoustic phenomena at high pressure is critical to the modeling of planetary dynamics, seismic events, and chemistry in extreme environments. Here we present the results of experiments using ultrafast laser excitation and detection of shock waves starting from high precompression (10s GPa) in a standard diamond anvil cell (DAC) with transient single shot shock pressures > 10 GPa. Using ultrafast interferometry, we directly detect surface motion with ~nm spatial resolution and ~ps time resolution. Such experiments enable examination of shock waves with significant strain starting at high ambient pressure using a convenient and relatively inexpensive apparatus. Ultrafast time resolution enables the observation of shock-induced chemistry on the scale of a picosecond shock rise. Furthermore, standard DACs can reach 100s GPa precompression, enabling the examination of phase transitions and chemical reactions starting from a wide range of thermodynamic initial conditions.

2:00PM

Session K1 Poster Session II: 2:00 pm - 5:00 pm Morial Convention Center Exhibit Hall A

K1.00001 SUPERCONDUCTIVITY —

K1.00002 Crystal Structure and Superconductivity of FeSr$_2$(Y,Nd)(Cu,Zn)$_2$O$_{6-δ}$δ. WUERNISHA TUERXUN, International Center for Materials Nanoarchitechtonics (MANA), National Institute for Materials Science (NIMS), Japan, TAKASHI MOCHIKU, Superconducting Materials Center, NIMS, YOSHIKATA HATA, Department of Applied Physics, National Defense Academy, AKINORI HOSHIKAWA, Ibaraki University, YOSHITAKA MATSUSHITA, Quantum Beam Center, NIMS, HIROKI FUJII, Superconducting Materials Center, NIMS, HIROSHI YASUOKA, Department of Applied Physics, National Defense Academy, HIDEAKI KITAZAWA, (1) Quantum Beam Center, (2) MANA, NIMS — We have prepared the polycrystalline samples of FeSr$_2$Y$_{0.75}$Nd$_{0.25}$(Cu$_{1-x}$Zn$_x$)$_2$O$_{6-δ}$δ solid solution system ($x=0,0.01,0.02,0.05$) to investigate the Zn substitution effects. The DC magnetization measurement results showing the samples exhibiting decreased in $T_c$ while increasing the Zn content, $x$, and the superconductivity was disappeared around $x=0.05$. Crystal structure has been analyzed by using X-ray and neutron powder diffraction data. The relation between the superconductivity and crystal structure is discussed based on the experimental results.

K1.00003 DC Magnetization and Growth of Heavy-Fermion Superconductor CeCoIn$_3$ and CeIn$_3$ Crystal. TESFAYE GEBRE, National High Magnetic Field Laboratory, ERIC PALM, STANLEY TOZER, TIM MURPHEY, JU-HYUN PARK, NHMF, JASON COOLEY, Los Alamos National Laboratory — The superconducting and magnetic state in heavy-fermion intermetallic compounds provides a promising realm of materials to study quantum critical behavior. Single crystals of the heavy-fermion superconductors CeCoIn$_3$ and CeIn$_3$, synthesized from the pure material using an excess of indium, are typically grown by flux technique. The details of the flux-growth technique used to grow CeCoIn$_3$ and CeIn$_3$ and the result of DC magnetization and transport measurements performed in the temperature range 1.9K to 100K will be reported.

1Work was supported by DOE DE-FG52-06NA26193, NSF Cooperative Agreement No. DMR-0084173, and the State of Florida

K1.00004 Superconducting Properties of Al-Eu Alloys. J. P. BYCHOWSKI, A. ORLOV, G. SNIDER, S. T. RUGGIERO, University of Notre Dame — We discuss the superconducting properties of Al-Eu alloys with Eu concentrations in the range of 0-5000ppm. The electron-transport and tunneling properties are discussed in the context of Abrikosov-Gor’kov pair-breaking and Kaiser resonant-scattering theories. This complements previous work on the Al-Mn system.
K1.00005 New Superconducting Material: Mg$_2$SnX (X = C, B)\(^1\), ANTONIO JEFFERSON MACHADO, Departamento de Engenharia de Materiais - Escola de Engenharia de Lorena - USP, BRUNO DE GODOI CURATTI, AUSDINIR DANilo BORTOLOZO, CARLOS ALBERTO DOS SANTOS, DEMAR TEAM — In the Mg-Sn system, there is only one intermetallic phase of Mg$_2$Sn composition. This intermetallic phase crystallizes in a cubic symmetry with prototype CaF$_2$ structure, named anti-fluorite. About three years ago, our group reported the existence of superconductivity in the Mg$_2$Sn intermetallic phase with a superconducting critical temperature close to 35 K \([1]\). In this intermetallic phase the boron atoms occupy the interstitial sites available in the structure. This work shows that, besides boron atoms, carbon also can occupy the interstitial sites in the same structure and can also induce superconductivity in the system with high critical superconducting temperature. This conclusion is sustained by resistivity, magnetization, and X-ray diffraction measurements. This report is based upon work supported by FAPESP (2005/01257-9). \([1]\) B. Ferreira, C. M Franco, C. A. M. dos Santos, D. Rodrigues Jr., L. Ghivelder, and A. J. S. Machado; Phys. C 408- 410, 148 (2004)

\(^1\)This report is based upon work supported by FAPESP (2005/01257-9).

K1.00006 New superconductor of the M$_2$AX family with Ti$_2$GeC composition, , A.D. BORTOLOZO, O.H. SANT’ANNA, C.A.M. DOS SANTOS, A.J.S. MACHADO, Departamento de Engenharia de Materiais EEL USP - Lorena Brazil. Polo Urbo Industrial Gleba AI-6 P.O. BOX 116 12600-970. — In this work the Ti$_2$GeC phase is investigated by x-ray diffraction, magnetic and resistivity measurements. Polycrystalline samples with nominal compositions Ti$_2$GeC were prepared by solid state reaction. The samples were encapsulated under argon and heat-treated at 1100°C for 240 hours. X-ray powder diffractograms suggest that all peaks can be indexed with the hexagonal phase of Cr$_2$AlC prototype. The electrical resistance as a function of temperature for the Ti$_2$GeC reveals a standard metal like behavior when this material is cooled from the heat treatment under equilibrium conditions. However, magnetic measurements display diamagnetic behavior close to 9.5K. On the other hand, when the Ti$_2$GeC phase is submitted a rapid quenching the R(T,B) curve shows superconducting critical temperature close to 9.5K without applied magnetic field. The magnetoresistance data with applied magnetic field suggests bulk superconductivity. In spite of the great number of compounds which belong to this family, superconductivity has been reported for five cases. So, this work sustains the idea of the existence of a new class of superconducting materials that crystallizes in the Cr$_2$AlC prototype.

K1.00007 Search for Magnesium Diboride like Binary Superconductors\(^1\), O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies[TCST], Abuja FCT, NIGERIA — Efforts to create compounds iso-electronic and iso-structural with magnesium diboride and also superconducting have so far met with limited success. Doping the Mg-site or the B-site have also not yielded higher transition temperatures. They have either been non-superconducting or have lower transition temperatures, Tc. Searching for magnesium diboride-like compounds using the electronegativity of MgB$_2$ (1.7333) has yielded a rich family of potential superconductors. The search has been facilitated using the recently designed ElectroNegativity Spectrum Maps [ENSMaps] of binary systems A$_x$B$_{1-x}$. Here we display the potential families. Using the relationship between Tc and atomic mass, we estimate the transition temperatures of the most likely Mg$_2$-like binary superconductors. We also suggest materials that can be doped to give an electronegativity of 1.7333.

\(^1\)with research support from Mr. Ferguson Uzoma and Institute for Superconducting and Electronic Materials [ISEM], Wollongong NSW Australia

K1.00008 Study of the Pseudogap in Y$_1-x$Ca$_x$Ba$_2$Cu$_3$O$_{7-d}$ Superconductor, EDWIN HERRERA, HECTOR CASTRO — The generic phase diagram of doping vs. temperature for High Temperature Superconductors (HTSC) presents in the underdoped region a zone called Pseudogap (PG). The analysis of this region is very interesting since it is believed that it is deeply related, and therefore can help us understanding better the superconductive (SC) transition. Different theories exist up to now which try to explain the origin of the PG and its influence on the SC transition. Some of them see the PG as a precursor of the superconducting gap, while others see it as a competing phenomenon which retards the SC transition. In the present work we analyze resistivity measurements in bulk samples of the high temperature superconductor Y$_1-x$Ca$_x$Ba$_2$Cu$_3$O$_{7-d}$, for different concentrations of calcium (x) and oxygen (d), and its influence on the PG zone. We discuss our results on the light of some of these theories.

K1.00009 MaxEnt-MuSR study of GdBCO: potential precursor effects, J. WONG, T. SONGATIKAMS, R. NORRIS, C. BOEKEMA, San Jose State University, WISE@SJSU COLLABORATION — We analyze muon-spin resonance (muSR) data of underdoped (Tc = 81 K) and optimal doped (Tc = 93 K) superconducting GdBCO showing different precursor effects. \([1]\) Precursors refer to anomalous behavior seen just above Tc. Transverse field muSR data recorded at 1 kOe, RT, and 100 K were analyzed by Maximum Entropy. MaxEnt determines the frequency (i.e. magnetic field) distribution from the muSR time series. \([2]\) Two Lorentzians fit the frequency signals much better than two Gaussians, one Lorentzian, or one Gaussian. Thus, in GdBCO the muon probes dynamic fields, caused by muon motion and/or magnetic fluctuations. The number of Balmer (muon-stop) sites with magnetic field) distribution from the muSR time series. \([2]\) Two Lorentzians fit the frequency signals much better than two Gaussians, one Lorentzian, or one Gaussian. Thus, in GdBCO the muon probes dynamic fields, caused by muon motion and/or magnetic fluctuations. The number of Balmer (muon-stop) sites [1] has been confirmed. Zero-field muSR curve fitting studies [1] showed irregularities in asymmetry and muon-spin relaxation just above Tc. We apply MaxEnt to these ZF GdBCO data to search for magnetic precursor effects. Research is supported by DOE-LANL and WISE@SJSU. \([1]\) Dawson et al, J Appl Phys 64 (1988) 5809; \([2]\) Lee et al, J Appl Phys 95 (2004) 6906; also at scitation.aip.org.

K1.00010 The enhanced high Tc superconductivity by ordering dopant, CHANGQING JIN, Q.Q. LIU, W.B. GAO, H. YANG, L.X. YANG, Y. YU, R.C. YU, Institute of Physics, Chinese Academy of Science, China, S. UCHIDA, Department of Physics, University of Tokyo, Japan — We discuss the high pressure improvement on superconducting transition temperature (Tc) related to ordering apical oxygen layer of a high temperature superconductor (HTS). This study became available in the high pressure synthesized Sr$_2$Ti$_2$O$_7$ superconductor with K$_2$NiF$_4$ structure showing so far rarely formed partially occupied ?apical oxygen? which also act as the dopant of the HTS. The well-defined links between Tc and modulated structures suggests that optimizing the ordering at apical oxygen layer outside CuO$_2$ plane is a promising way to further enhance Tc.

K1.00011 Mo$_2$BC: Chemical and External Pressure Effects\(^1\), R. FALCONI, DACB-Universidad Juarez Autonoma de Tabasco, R. ESCAMILLA, R. ESCUDERO, IIM-Universidad Nacional Autonoma de Mexico — The intermetallic Mo$_2$BC is a superconductor with a Tc = 6.6 K and a crystalline face centered orthorhombic structure. Chemical pressure generated by changing the carbon concentration decreases Tc in a non monotonic rate. Complete elimination of carbon, changes the crystalline structure from orthorhombic to body centered tetragonal, and reducing Tc to about 5.8 K. At ambient pressure the compound presents a minimum in the resistivity at 50 K, which could be related to a Kondo anomaly. In polycrystalline samples we applied external pressures up to 4.8 GPa with a diamond anvil cell, which induced negative changes in the superconducting transition at a rate dTc/dP = - 0.03 K/GPa. These results will be discussed in terms of the electronic band structure.

\(^1\)Acknowledgements: (R. F.) Thanks SEP-Promepe 20050643 UJATAB-CA175.
K1.00012 Unconventional Metallic Phase of the Quasi Two-Dimensional Organic Superconductors. EDDY YUSUF, B.J. POWELL, R.H. MCKENZIE, Physics Department, University of Queensland, Brisbane 4072, QLD, Australia. — We show, by analyzing previously published nuclear magnetic resonance (NMR) data, that there are large antiferromagnetic fluctuations above $T_{\text{NMR}} \approx 50$ K in the metallic phase of $\kappa-(ET)_2X$ family of organic charge transfer salts. The proximity of the metallic phase to the antiferromagnetic Mott insulating phase and the d-wave superconductivity are thought to be the origin of the large antiferromagnetic fluctuations. The antiferromagnetic correlation lengths are estimated to be several lattice constants at $T_{\text{NMR}}$, which place the materials between the isotropic triangular lattice and the square lattice. For materials close to the Mott insulating phase the nuclear spin relaxation rate per unit temperature, Knight shift and Körringa ratio all decrease significantly with decreasing temperature below $T_{\text{NMR}}$, inconsistent with the renormalized Fermi liquid picture previously thought to be the correct description of the low temperature metallic phase in these materials. One plausible explanation is that a pseudogap, similar to that observed in the underdoped cuprate superconductors, opens up in the density of states below $T_{\text{NMR}}$. Such a pseudogap has recently been predicted to occur in the dimerised organic charge transfer salts materials by the resonating valence bond (RVB) theory.

K1.00013 Photoemission Spectroscopy on the System of Noncentrosymmetric Lithium Ternary Borides. RIKIYA YOSHIDA, IZUMI HASE, KOZO OKADA, HIROYUKI TAKEYA, KAZUTO HIYATA, TAKAYUKI MURO, HIROYUKI OKAZAKI, MITSUTOSHI TAJIMA, MASAKI HIRAI, YUJII MURAOKA, TAKAYOSHI YOKOYA, Okayama University — We performed x-ray photoemission spectroscopy at BL27SU of SPring-8 on polycrystalline samples of Li$_2$Pd$_3$S$_3$, Pd$_3$B$_2$ and Li$_2$Pd$_3$B$_2$ prepared by the arc melting method. We also employed a polycrystalline platinum plate commercially available for comparison. We also performed the calculation of valence band structure of Li$_2$Pd$_3$B$_2$ using full-potential augmented plane wave method with local density approximation. Our experimental data on the samples and the previous photoemission study on Li$_2$Pd$_3$B$_2$ support that electron correlations do not play an important role in them.

3The x-ray photoemission experiments were performed at SPring-8 under the proposal number of 2007B1519. One of the authors (R. Y.) thanks Grant-in-Aid for Attractive Education in Grant-in-Aid for Attractive Education in Graduate School.

K1.00015 Magneto-thermal instabilities in irradiated high density MgB$_2$ compound. E. VERDIN, Dpto. Fisica- U. Sonora, Mexico, A. DURAN, D.H. GALVAN, CCMC-UNAM, Mexico, E. IEM-UNAM, Mexico, M.B. MAPLE, DIP-PAP-U.C.-La joya-U.S.A., F. MORALES, R. ESCUDERO, IIM-UNAM, Mexico — The effects of irradiation with low dosages of $\gamma$-rays, protons and electrons on the magnetization and critical current density of MgB$_2$ bulk samples were studied. Magnetic susceptibility measurements present a transition temperature with diamagnetic signal at $\approx 38.5$ K. Magneto-thermal instabilities as flux jumps are observed in the magnetization hysteresis loops below 23 K, for all samples. The flux jump behavior is independent of the irradiation. The number of flux jumps decreases as the temperature increases. The magneto-thermal instabilities observed is a competing process between the Lorentz and pinning forces that depend on the bath temperature as well as on the defect density that influence the current density. The field dependence of the critical current density, $J_c$, was evaluated using the Bean’s model for different temperatures (from 2, 10, 15, and 20 K). The results show instabilities in the critical current, $J_c$, below 10 K as a consequence of the flux jumps events observed in the isothermal magnetization curves. In this presentation we will analyze the influence of the flux jumps on the critical currents densities.

K1.00016 Observed magnetism and its field dependence in c-axis-oriented YBCO vortex states. C. BOEKEMA, San Jose State University, C. TEICHGRAEBER, UC Berkeley, WISESJSU COLLABORATION — Muon-spin-resonance ($\mu$SR) data of c-axis-oriented YBCO [1} vortex states are analyzed to determine the field dependence of observed AF magnetism. Field distributions are obtained from $\mu$SR data using Maximum-Entropy (ME). We found [2} that well below $T_c$, YBCO vortex signals are best fitted by a Gaussian and a Lorentzian; the latter indicating AF in and near the vortex cores. The field dependence of the AF Lorentzian width is about linear. [2} ME-$\mu$SR analysis of c-axis-oriented YBCO data also suggests a field direction dependence, pointing toward 3-d magnetism. Our results show contraditions to curving fit and FFT results. [1} An LSCO neutron study agrees with AF 3-d field-induced AF. [3} An AF presence in and near vortex cores supports theories predicting a magnetic origin for cuprate superconductivity. [3, 4} Research supported by NSF-REU, DOE-LANL and WISE-SJSU. [1] Lichti et al, Hpf Int’s 63 (1990) 73; [2] Boekema et al, Physica C460-462 (2007) 1255 and ref’s therein; [3} Lake et al, Nature Materials 4 (2005) 658; [4} Chen, Zhang et al, Phys Rev B 67 (2003) 22051.

K1.00017 Magnetization, Creep, and Flux Pinning in YBa$_2$Cu$_3$O$_{7-x}$ Thin Films with Nanoscale Pinning. M.D. SUMPTON, Ohio State University, T.J. HAUGAN, P.N. BARNES, Air Force Research Laboratory, C. VARANASI, University of Dayton Research Inst. — Critical current and flux pinning have been studied for YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) thin films with Y$_2$BaCuO$_5$ (211) precipitates introduced as layers and as random distributions. Magnetically determined critical current density ($J_c$) was fit to $J_c \propto B^{\alpha}$ and values of $\alpha$ were suppressed from the control sample values of $\alpha = 0.5$ to lower values for pinned samples, reaching as low as $\alpha = 0.2$ for the layer pinned 211 sample at low temperatures. $U/J$ vs $J$ curves were extracted from M-H measurements with various ramp rates, at temperatures from 4.2 K to 77 K for pinned and control samples. Direct magnetization decay measurements were made for the 211 layer pinned sample and good agreement was seen with ramp rate derived results. Values of $\mu \approx 0.6-0.8$ were seen for all samples, while $\mu \approx 0.4$ for control samples, 0.1 for layer pinned samples, and 0.0-0.4 for the random pinned samples. The values of $\mu$ and $\nu$ extracted were inconsistent with 2-D pinning behavior in all cases, even though the layer spacing in the layer pinned sample is smaller than the calculated collective correlation length. While the layer pinned sample is clearly in the collective pinning regime, the artificial defects in the random pinned sample may be in the isolated strong pinning regime.

K1.00018 Oxidation of MgB$_2$ Thin Films. J. READ, Cornell, Y. CUI, Penn State, B. MOECKLY, Superconductor Technologies, J. SHU, Cornell, X. XI, Penn State, R. BUHRMANN, Cornell — We report on x-ray photoelectron spectroscopy studies of the surface oxides of high quality MgB$_2$ thin films grown both by reactive evaporation [1] and by hybrid chemical physical vapor deposition [2]. Depending upon the treatment of the MgB$_2$ surface after deposition, the oxide can contain both magnesium and boron, with a substantial variation in the Mg:B ratio. Brief high temperature ($T \geq 400 {^\circ}C$) exposure of the MgB$_2$ surface to even near ultra-high-vacuum conditions, results in the formation of a thin mixed oxide (Mg$_x$B$_{1-x}$O$_y$) and subsurface layer of elemental B due to the greater reactivity of Mg. As a result of the higher mobility of the Mg cations, prolonged exposure to the background ambient additionally results in a progressively thicker MgO surface oxide layer, and in a larger elemental B subsurface component. The surface oxide formed at $\approx$38.5 K. Magneto-thermal instabilities as flux jumps are observed in the magnetization hysteresis loops below 23 K, for all samples. The results show instabilities in the critical current, $J_c$, below 10 K as a consequence of the flux jumps events observed in the isothermal magnetization curves. In this presentation we will analyze the influence of the flux jumps on the critical currents densities.
K1.00019 Deposition temperature dependence of YBCO transport properties, JIE WANG, J.H. KWON, J. YOON, H. WANG, Texas A&M University, T.J. HAUGAN, F.J. BACA, N.A. PIERCE, P.N. BARNES, Air Force Research Laboratory — In this paper, we report a strong correlation between the stacking fault (SF) density and the critical current density of YBa$_2$Cu$_3$O$_7$-(δ)YBCO thin films in an applied field (Jcin-field). High quality superconducting YBCO thin films (thickness ~300 - 350 nm) were deposited on SrTiO$_3$ (STO) and LaAlO$_3$ (LAO) substrates using a pulse laser deposition (PLD) technique. We found that the Jcin-field increases as the deposition temperature increases (775°C - 825°C) for the samples grown on both STO and LAO substrates. Detailed microstructural studies including cross-section transmission electron microscopy (TEM) and high resolution TEM were conducted for all the films deposited on STO substrates. The YBCO SF density increases from ~ 4.0 x10$^5$/cm to ~1.2 x10$^6$/cm as the deposition temperature increases from 775°C to 825°C. An interesting linear relation is observed between the SF density and the Jcin-field value, which suggests that the YBCO SF density plays an important role in the YBCO in-field transport performance.

K1.00020 Fluctuation Nernst-Ettingshausen Effect above Ordinary/Quantum Superconducting Transition, ANDREI SERGEEV, SUNY at Buffalo, MICHAEL REIZER, VLADIMIR MITIN, SUNY at Buffalo — A problem of the definition of the heat transferred in thermomagnetic phenomena has been well realized in the late sixties, but not solved up to date. Ignoring this problem, numerous recent theories grossly overestimate the thermomagnetic coefficients in strongly interacting systems. Here we develop a gauge-invariant microscopic approach, which shows that the heat transfer should include the energy of the interaction between electrons and a magnetic field. We also demonstrate that the surface currents induced by the magnetic field transfer the charge in the Nernst effect, but do not transfer the heat in the Ettingshausen effect. Only with these two modifications of the theory, the physically measurable thermomagnetic coefficients satisfy the Onsager relation. We critically revised the Gaussian fluctuation theory above the ordinary/quantum superconducting transition and show that the gauge invariance uniquely relates thermomagnetic phenomena in the Fermi liquid with the particle-hole asymmetry.

K1.00021 Flux-Flow noise in YBCO thin films in the normal region, transition and superconducting state, PAULA GIRALDO, HECTOR CASTRO — The dynamic of vortexes inside type II superconductor thin films in the mixed state, is that, under their critical temperature and immersed in a DC magnetic field below its critical value, can be studied by means of the measurement of flux-flow noise, before the transition, during it and in the superconducting state. We measure the fluctuation in the voltage signal in the pseudogap region for an YCaBaCuO thin film, and compare it with the response in the other two regions. The response for overdoped and underdoped samples is compared with the response of optimal doped samples.

K1.00022 Phase diagram and vortex dynamics in superconducting spherical nanoshells, JACQUES TEMPERE, TFVS, Universiteit Antwerpen, VLADIMIR GLADILIN, INPAC, Katholieke Universiteit Leuven, ISAAK SILVERA, Lyman Laboratory of Physics, Harvard University, JOZEF DEVREESE, TFVS, Universiteit Antwerpen, VICTOR MOSCHCHALOV, INPAC, Katholieke Universiteit Leuven — Curving a superconducting film into a spherical shell changes its vortex-related properties drastically due to topological constraints. The interplay between the Lorentz force due to an applied field and the vortex superflow will force vortices away from the equator (leaving an equatorial “Meissner band”) and towards the poles, where they may coalesce to form giant or ring-like vortexes. Using the time-dependent Ginzburg-Landau equations adapted for the spherical geometry, we derive the phase diagram and identify where, as a function of the applied magnetic field, the shell thickness and the shell radius, different vortex phases occur. We also examine the dynamics of the decay of giant and ring-like vortices into a vortex lattice, when the magnetic field is adapted so that a phase boundary is crossed. Moreover, we show that the vortex dynamics are insensitive to moderate imperfections in the shell: effects due to topological constraints can overcome the pinning potential due to imperfections. This robustness, together with the tunability of the phase diagram through a limited set of controllable parameters, makes superconducting nanoshells uniquely suited for the study of vortex states.

K1.00023 Out of equilibrium phase dynamics in ferromagnetic Josephson junctions, IVANA PETKOVIC, MARCO APRILI, Laboratoire de Physique des Solides, Univ. Paris-Sud, CNRS, UMR 8502, F-91405 Orsay Cedex, France — With a pump-probe measurement performed below 1K, we probe the switching mechanism of strongly underdamped ferromagnetic Josephson junctions in the classical limit. At equilibrium or for slow sweeps, we observe that the switching is governed by thermal fluctuations, as expected. When the sweep frequency is comparable to the inverse phase relaxation time, we observe premature switching due to phase bifurcation. From the frequency dependence of the switching probability we deduce the phase relaxation rate τ = 1/RC, where R is the quasiparticle resistance and C the junction capacitance. Moreover, we observe a peculiar scaling of the Fiske steps (resonances between the Josephson phase and the electromagnetic cavity modes) with the junction length: the resonance frequencies are not multiples of the inverse junction length, but present a finite offset. We attribute this offset to the high frequency ferromagnetic susceptibility.

K1.00024 Macroscopic quantum tunneling in a damped Josephson junction coupled to a nanomechanical resonator, JOSHUA SCHIFFRIN, Carnegie Mellon University, BRAD TREES, YASER HELAL, Ohio Wesleyan University, BRIAN SILLER, University of Illinois at Urbana-Champaign — Motivated by work in the field of quantum computation, we studied the tunneling rate in a damped Josephson junction (JJ) coupled to a nanomechanical resonator. The Josephson phase difference was treated as the coordinate of a particle trapped in a metastable cubic potential well, and the resonator was considered to be a simple harmonic oscillator. The damping on the system by the environment was modeled as two reservoirs of simple harmonic oscillators, one of which was coupled to the JJ, and the other coupled to the resonator. We found that damping the JJ suppresses the tunneling rate, a result already predicted by theory and verified by experiment for a single JJ. We also find that increasing the coupling strength between the JJ and the resonator suppresses the tunneling rate, while adding damping to the resonator actually enhances the tunneling rate. These results are important, as a full understanding of the tunneling rate’s dependence on system parameters is essential for the proper operation of quantum bits.

K1.00025 Suppression of quantum fluctuations in a Josephson junction coupled to a nanomechanical resonator, YASER HELAL, BRAD TREES, Ohio Wesleyan University, JOSHUA SCHIFFRIN, Carnegie Mellon University, BRIAN SILLER, University of Illinois at Urbana-Champaign — The quantum mechanical properties of a Josephson junction (JJ) in parallel with a nanomechanical resonator were studied. The JJ phase difference was treated as a “particle” trapped in a quadratic potential well, which was used to approximate the well-known tilted washboard potential of the junction. When coupled to the resonator, the square of the uncertainty in the position of the JJ “particle” was suppressed, i.e. quantum fluctuations of the JJ were reduced by the resonator. The uncertainty principle was obeyed by the system, in that the square of the uncertainty in the JJ’s momentum was enhanced with resonator coupling. We also included the effects of environmental damping. Damping the junction enhanced the suppression of quantum fluctuations beyond that due to resonator coupling alone. Damping the resonator, however, suppressed the effect of JJ-resonator coupling and thus resulted in less suppression of quantum fluctuations. Preliminary results for the effects on quantum fluctuations of a weak nonlinear term in the JJ’s potential energy have also been obtained.

1Work supported by the National Science Foundation (REU/RET grant #0648751) and Ohio Wesleyan University.

3Work supported by the National Science Foundation (REU/RET grant #0648751) and Ohio Wesleyan University.
Comparisons to experiment.

A new retrapping mechanism for fluxons, related to the coupling of the junctions in the array, has been identified. We present results from the simulations and determination of the transition rate of the fluxon from its pinned state to a running state. We simulate the classical RCSJ equations of motion for a 9-junction. Simulations of switching current measurements have been performed in order to support experimental work in our group. Switching current measurements allow incoherent electron charge pairing above $T_c$ and pair coherency with spin condensation below $T_c$. These ideas may also be linked to recent atomic scale tunneling experiments in La cuprates on nucleation of pairing pseudogaps and microscopic inhomogeneities in a real space.

KENNETH SEGALL, NIKHIL FERNANDES — We present a numerical study of the dynamics of fluxons trapped in a parallel array of Josephson junctions.

KENNETH SEGALL, NIKHIL FERNANDES —

Equation (1)

\[ \text{Equation (2)} \]

1. Equation (3)

2. Equation (4)

Funding from NSF Grant DMR 0509450

3. Equation (5)

Funding from NSF Grant DMR 0509450

4. Equation (3)

K1.00027 Exact thermodynamics of phase separation and pairings in Hubbard nanoclusters — ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University Los Angeles, GAYANATH FERNANDO, TUN WANG, KALUM PALANDAGE, Department of Physics, University of Connecticut, JIM DAVENPORT, Computational Science Center, Brookhaven National Laboratory — The exact numerical diagonalization and thermodynamics in an ensemble of small Hubbard nanoclusters reveal intriguing insights into the phase separation, charge and spin pairings, Bose condensation and ferromagnetism in nanometer scale. The phase diagram off half filling strongly suggests the existence of electron pairing, superparamagnetism and saturated ferromagnetism in small nanoclusters driven by electron repulsion and doping. Rigorous criteria for the existence of charge and spin pairings in the ground state and corresponding crossovers at finite temperatures are formulated. The phase separation and electron pairing, monitored by a magnetic field and electron doping, surprisingly resemble phase diagrams in the family of doped high $T_c$ cuprates. Exact theory provides incoherent electron charge pairing above $T_c$, and pair coherency with spin condensation below $T_c$. These ideas may also be linked to recent atomic scale tunneling experiments in La cuprates on nucleation of pairing pseudogaps and microscopic inhomogeneities in a real space.

K1.00028 Ferromagnetic Pairing Ground States on Two-Coupled Chains — AKINORI TANAKA, Ariake National College of Technology — Recently, ferromagnetic superconductivity was discovered in ZrZn$_2$, UC$_2$Ge$_2$ and UB$_2$Ge$_2$. Microscopic explanation of this phenomenon is a challenge in theoretical physics, but the problem is rather subtle and difficult, since we have to treat rotational symmetry breaking of spin and electron-pair condensation simultaneously. At the present stage, it is expected that a simple concrete model exhibiting both ferromagnetism and electron-pair condensation, even if it has somewhat artificial aspects, will shed light on understanding of mechanisms of ferromagnetic superconductivity. Here we report an extended Hubbard model on two chains which has fully polarized pairing ground states. The Hamiltonian consists of intra-chain electron-hopping, on-site repulsion, inter-chain charge attraction and inter-chain ferromagnetic interaction terms. The following is shown in our model. In the case where the on-site repulsion term is vanishing, the model has degenerate ground states in which electrons form spin triplet pairs, and thus the ground states exhibit electron-pair condensation but do not exhibit ferromagnetism. When the on-site repulsion is added, the model has the unique (up to spin degeneracy) ground state in which ferromagnetism and electron-pair condensation coexist. We also present an extension of the model to higher dimensional cases.

K1.00029 Electron charge pairing and Nagaoka spin instabilities in nanoclusters — ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University Los Angeles, GAYANATH FERNANDO, KALUM PALANDAGE, Department of Physics, University of Connecticut, JIM DAVENPORT, Computational Science Center, Brookhaven National Laboratory — The electron pairings and magnetism in various frustrated Hubbard clusters is studied systematically with emphasis on under doping, magnetic field and temperature. Small clusters provide insight into charge-spin separation and thermal condensation of electron charge and spin degrees [1]. The spin saturated phase in so called Nagaoka state is found equivalent to ferromagnetic Mott-Hubbard like insulator with spin pairing gap, while non maximum spin ground state is of BCS-like metallic origin with equal charge pairing and spin gaps. The calculated phase diagrams resemble a number of spatially inhomogeneous coherent and incoherent paired phases seen in nanometer scale in high $T_c$ cuprates, fullerene molecules, Co and Nb nanoparticles. [1] A. N. Kocharian, G. W. Fernando, K. Palandage, Tun Wang and J. W. Davenport, Phys. Rev. B 62, 8671 (2000).

K1.00030 Dynamic Response to On/Off Signals in Nano Junctions — ZHANYU NING, McGill University, YU ZHU, JOSEPH MACIEJKO, JIANG WANG, HONG GUO, HONG GUO TEAM, JIANG WANG TEAM — We report the implementation of the time-dependent nonequilibrium Keldysh Green’s function theorem (TD-NEGF). It provides a promising way to study the transient transport dynamics in nano devices by first principles calculation. Very importantly, we derive an efficient technique to overcome the singularity problem in the integration of spectrum function. The reliability of this method is carefully checked by a one-dimension chain model with the analytical solution. We then perform the ab-initio calculation in a realistic molecular junction (Al-Benzene-Al). The current dynamic response arises after applying an “upward” or “downward” step pulse, which predicts a characteristic timescale in transport dynamics of nano systems.

K1.00031 One-dimensional fermion pairing — RAFAEL MENDOZA, Posgrado en Ciencias Fisicas, UNAM, M. DE LLANO, Instituto de Investigaciones en Materiales, UNAM, M. FORTES, M.A. SOLIS, Instituto de Fisica, UNAM, Mexico — We study fermion pairing in a one-dimensional fermion gas at $T = 0$ interacting via a generalized two-body attractive, separable interaction [1] where the effective range was varied from zero (delta potential) to infinity. The binding energy of fermion pairs with zero center-of-mass momentum increases as a function of the interaction strength and decreases as a function of the interaction range for a given strength. Fermion pairs with finite, nonzero center-of-mass momentum have an energy dispersion relation that exhibits two excitation branches: One phonon-like for low momentum which, for weak coupling, can disappear before the second, roton-like excitation appears for values of the momentum larger than $2k_F$ and only above a minimum threshold interaction strength value. The interaction range has the effect of privileging the quadratic over the linear relation dispersion as it goes from short to long range. This study completes a trilogy initiated for 3D [2] and later for 2D [3].


1. We acknowledge the partial support from grant PAPIIT IN111405-3 and CONACYT 4324-F.

2. Funding from NSF Grant DMR 0509450.
K1.00033 Signatures of Kosterlitz-Thouless behavior in the superfluid density of anisotropic layered superconductors, LARA BENFATTO, Centro Fermi and University of Rome “La Sapienza”, CLAUDIO CASTELLANI, University of Rome “La Sapienza”, THIERRY GIAMARCHI, University of Geneva — In quasi-two-dimensional (2D) systems, as thin films of He or of superconductors, the superfluid transition is expected to be driven by phase fluctuations, according to the Kosterlitz and Thouless (KT) theory. However, signatures of KT vortex-antivortex phase fluctuations should be observable, at some energy scale $T_d$, also in strongly anisotropic layered superconductors, where quasi-2D behavior arises due to a small Josephson coupling between neighboring planes. While in the 2D case $T_d$ is uniquely identified by the KT temperature $T_{KT}$ where the universal jump of the superfluid density is observed, in the layered case such universality is lost. Here we show this effect by means of a renormalization-group analysis of a layered version of the sine-Gordon model, appropriate to describe the occurrence of KT physics in layered superconductors. We find that in the presence of a finite interlayer coupling $T_d$ is controlled by the vortex-core energy, and can be significantly larger than the 2D scale $T_{KT}$. When applied to the superfluid-density behavior in cuprate superconductors these results allows us to determine a non-trivial behavior of the vortex-core energy in these systems. L.Benfatto, C.Castellani and T.Giamarchi, Phys. Rev. Lett. 98, 117008 (2007).

K1.00034 Fermi surface arcs and the infrared conductivity of underdoped YBa$_2$Cu$_3$O$_{6.5}$, JUNGSEEK HWANG, University of Florida, JULES P CARBOTTE, THOMAS TIMUSK, McMaster University — Using recent finding, that the electronic states lost below the pseudogap energy ($\Delta$) are recovered in the energy region immediately above it, we analyze the in-plane far infrared conductivity data in underdoped ortho$\beta$YBa$_2$Cu$_3$O$_{y.5}$, and are able to find evidence for the opening of a pseudogap on part of the Fermi surface with the remaining ungaped piece proportional to the temperature. These results are similar to recent angle-resolved photoemission spectroscopy data in underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8-\delta}$.

1 This work has been supported by the Canadian Natural Science and Engineering Research Council (NSERC) and the Canadian Institute for Advanced Research (CIAR).

K1.00035 Ultrafast Carrier Dynamics of YBCO Films with Various In-plane Orientations Investigated by Pump-probe and Terahertz Spectroscopy, SHYH-SHIH PAI, ZEN-CHI LIN, PAO-AN LIN, CHENG-CHUNG CHI, INSTRUMENT TECHNOLOGY RESEARCH CENTER, NATIONAL APPLIED RESEARCH LABORATORIES, TAIWAN, ROC TEAM, INSTITUTE OF PHOTONICS TECHNOLOGIES, NATIONAL TSING HUA UNIVERSITY, TAIWAN, ROC TEAM, DEPARTMENT OF PHYSICS, NATIONAL TSING HUA UNIVERSITY, TAIWAN, ROC TEAM — In this study, we focus on the terahertz (THz) and optical responses of superconducting YBa$_2$Cu$_3$O$_{6-\delta}$ (YBCO) films with various in-plane orientations. We report results and analyses of THz time domain spectroscopy and time-resolved photoinduced reflectivity experiments on four in-plane oriented superconducting YBCO films grown on yttria-stabilized zirconia substrates. Our study of the transmissions of THz time domain spectroscopy indicates a higher value of conductivity at room temperature for the 0°-orientation films than the 45°-films. Using the optical pump-THz probe scheme, we observed combinations of positive and negative THz transmission transients relative to a thermal equilibrium level with different relaxation times of about 0.9 and 9.0 ps respectively for all samples containing 45°-domains. Possible physical mechanisms will be discussed.

K1.00036 Influence of oxygen orbitals on impurity states in superconducting cuprates, ALEXANDER KEMPER, HAI-PING CHENG, P.J. HIRSCHFELD, University of Florida — Recent STM studies have shown that the oxygen states play a hitherto unappreciated role in the inhomogeneous electronic structure of the CuO$_2$ plane. To gain some insight into these effects, we solve the Bogoliubov-de Gennes equations numerically for a 3-band Hubbard model with d-wave pair interaction. We consider the role of the various oxygen atomic orbitals in the in the formation of impurity bound states and magnetic moments in the presence of correlations described by the Hubbard U. Finally, we study the interference of many impurities.

3 This work was supported by DOE grants DE-FG02-97ER45600, DE-FG02-05ER46236 and DE-FG02-02ER45995 and by the University of Florida High Performance Computing center.

K1.00037 Nature of the superconductor-insulator transition in disordered thin films, YONATAN DUBI, Physics Department, University of California-San Diego, YIGAL MEIR, YSHAI AVISHAI, Department of Physics and The Ilse Katz Center for Meso- and Nano-Scale Science and Technology, Ben Gurion University, Beer Sheva 84105, Israel — Highly disordered superconducting (SC) thin films undergo a magnetic-field (B) driven superconductor-insulator transition (SIT) whose detailed nature is still not completely understood. Starting from a microscopic description, we analyze this SIT in disordered thin films, and demonstrate that disorder leads to the formation of islands where SC order is rather high. For weak disorder, increasing B eventually results in the vanishing of the SC order parameter, implying an insulating state. At higher disorder, however, increasing B suppresses correlations between phases of the SC order parameter in different islands, giving rise to a novel kind of SIT. One of the remarkable predictions of this study is that in the latter regime, there are still SC islands in the sample even on the insulating side. This outcome, which is consistent with pertinent experiments, explains the recently observed huge magneto-resistance peak in disordered thin films. It may also be relevant in attempts to explain the occurrence of pseudo-gap in under-doped high-Tc superconductors, which have recently been found to be intrinsically disordered.

K1.00038 Growth and properties of Wo3, NasWo3, and KxWo3 thin films, AKIO TSUKADA, SEUNG SAE HONG, RICHARD J. HAMMOND, THEODORE GEBALLE, MALCOLM BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University — We report optimization of thin-film growth conditions and films properties of Wo3, NasWo3, and KxWo3. Films are grown by pulse laser deposition and used as substrates are (100) LaAlO3 (a = 3.788 A) and (101) Y-ZrO2 (3.63 A). Growth temperature and oxygen pressure are varied from 600C to 300C and from 10 mTorr to 1000 mTorr, respectively. Wo3 are formed in monoclinic or tetragonal structure on LaAlO3 substrates. Films are insulators and temperature dependence of resistivity shows the variable range hopping with Coulomb interaction like behavior [resistivity is proportional to exp(1/T)^(1/2)]. On Y-ZrO2 substrates are (100) LaAlO3 (a = 3.788 A) and (111) Y-ZrO2 (3.63 A). Growth temperature and oxygen pressure are varied from 600C to 300C and from 10 mTorr to 1000 mTorr, respectively. Wo3 films are formed in monoclinic or tetragonal structure on LaAlO3 substrates. Films are insulators and temperature dependence of resistivity shows the variable range hopping with Coulomb interaction like behavior [resistivity is proportional to exp(1/T)^(1/2)]. Y-ZrO2 substrates are formed in mixed structure of hexagonal and tetragonal due to an epitaxial effect [(111) Y-ZrO2 substrate has hexagonal surface]. KxWo3 films are formed in mixed structure of hexagonal and tetragonal due to an epitaxial effect [(111) Y-ZrO2 substrate has hexagonal surface]. KxWo3 films are formed in hexagonal structure on both substrates. a- and c-axis oriented films are obtained on LaAlO3 and Y-ZrO2 substrates, respectively. KxWo3 films show superconductivity at Tc(onset) ~ 4 K and Tc(zero) ~ 2 K. This work is supported by Air Force Office of Scientific Research.

K1.00039 ABSTRACT HAS BEEN MOVED TO SESSION X11

K1.00040 Vortex phase diagram and electromagnetic anisotropy of cation composition controlled Bi2212 single crystals, JUN-ICHI SHIMOMURA, TAKANORI MAKISE, YOSHIKI KAGESHIMA, SHIGERU HIRIO, KOJI YASUDA, Department of Applied Chemistry, University of Tokyo — In the present study, vortex phase diagram and pinning properties of Bi2212 single crystals under H // c have been systematically studied as functions of cation and oxygen compositions, while these matters were well understood for slightly cation-nonstoichiometric samples almost ten years ago. We confirmed that cation stoichiometry largely affects vortex state and pinning strength. A particular crystal with a cation composition of nearly 2:2:1.2 “Bi2212” exhibited strong bulk pinning behaviors even in the high temperature region, resulting in disappearance of magnetic irreversible region below the first-order-transition (FOT) temperature of vortex state. In addition, entropy change of the vortex at FOT of “Bi2212” crystals was found to be apparently larger than that of conventional ones. On the contrary, Bi and Ca-rich and Sr-poor single crystals showed poor pinning behaviors with low irreversibility fields and critical current density. Systematic enhancement of in-plane anisotropy in resistivity, decreases in $\rho_c$ and increases of penetration depth with approaching the cation stoichiometric composition suggested that disordered crystal lattice due to partial substitutions of Bi and Ca for Sr-site, which is common for conventional Bi2212 single crystals, degraded superconducting properties of Bi2212.
**K1.00041** What is the vortex “transport entropy”?\(^1\) ANDREI SERGEEV, SUNY at Buffalo, MICHAEL REIZER, VLADIMIR MITIN, SUNY at Buffalo — Below the superconducting transition the large thermomagnetic effects in the type II superconductors are determined by magnetic vortices. These topological excitations are completely different from particle-hole excitations in the Fermi liquid and, therefore, the thermomagnetic effects do not require particle-hole asymmetry. Thermomagnetic effects in the vortex state are widely described in terms of the “transport entropy.” Despite of intensive theoretical and experimental investigations, this mysterious quantity is still in conflict with either the Onsager principle or the third law of thermodynamics [1]. We resolve this forty years enigma taking into account the magnetization current in the presence of the temperature gradient. Then contributions of superconducting currents of vortices are canceled in the Nernst effect, and, therefore, in agreement with the Onsager relation, both the Nernst and Ettingshausen phenomena originate solely from vortex cores. Finally, the transport entropy turns out to be by a factor of $4\ln(\lambda/\xi)$ smaller than that used in literature [1] ($\lambda$ is the magnetic field penetration depth, $\xi$ is the coherence length. For high-temperature cuprates this factor is $\sim 20$.


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**K1.00042** Variational Monte-Carlo investigation of gossamer-superconductivity, SIEGFRIED GUERTLER, FU-CHUN ZHANG, The University of Hong Kong, Department of Physics — Motivated by the interesting superconducting properties in layered organic materials, and the proposed gossamer superconductivity in this context, we performed variational Monte-Carlo simulations. We investigate a previously proposed model-Hamiltonian of a Hubbard-model with additional anti-ferromagnetic coupling term. We work on a square lattice with additional diagonal bonds and with a wave-function with partly projected double-occupanted states. Further factors for anti-fermagnetic states are introduced in our wave-function.

**K1.00043** Superconducting Mechanism in multi-walled Carbon Nanotubes, YONG-JIHN KIM, University of Puerto Rico — Recently Japanese group led by Haruyama [1] reported the significant enhancement of superconductivity, i.e., $T_c=12K$, in end-bonded Multi-walled Carbon Nanotubes. We can explain the enhancement by the electron confinement in the lateral direction, i.e., between the inner and outer cylinders, because electron density correlation enhances the phonon-mediated superconductivity. In other words, superconductivity in the (multi-walled) Carbon Nanotubes is due to the electron-phonon interaction and $T_c$ is enhanced due to the density correlation caused by the confinement. First, we use simple concentric rings to estimate the $T_c$ enhancement using the BCS theory. Next, we use the tight-binding model to calculate the $T_c$ increase more accurately. In this context, this experimental result is very similar to the enhancement of $T_c=15K$ in 4 angstrom single-walled Carbon Nanotubes by Tang et al. [2]. [1] I. Takesue et al., Phys. Rev. Lett., Vol. 96, 057001 (2006). [2] Z. K. Tang et al., Science, Vol. 292, 2462 (2001).

**K1.00044** Theoretical Investigation of Fermion Pairing in Three-band Extended Hubbard Model, PARTHA GOSWAMI, University of Delhi — We analyze for fermion pairing the two-dimensional extended Hubbard model (or d-p model) on a square lattice by a slave-boson method reported in a previous work\(^1\). The onsite coulomb repulsion between Cu d holes is assumed to be strong. The nearest-neighbor interaction in momentum space $U_{kq}$, introduced additionally, for transition from a momentum q to k is assumed to be separable and is expanded in terms of basis functions corresponding to $d_{xy}$ and $d_{x^2−y^2}$. The possibility of a mixed (s-d)-wave symmetry also exists for the spin degeneracy $N>|\lambda\rangle$ if boson field fluctuations are taken into consideration. For the hole doping ($\delta > 0$) case, the additional holes are expected to occupy oxygen sites. This implies that the renormalized charge transfer gap $\Delta_{xy}$ tends towards zero for $\delta > 0$. We find the approximate Fermi liquid behavior for $\Delta_{xy}$ once the pure $d_{x^2−y^2}$ wave singlet superconducting instability sets in; otherwise non-Fermi liquid behavior is the prevalent one. The charge and the spin ordering gaps appear in the single-particle excitation spectrum when $d_{xy}$ component is taken into account. The latter is expected to lead to the spin-pseudo-gap phenomenon in cuprates.

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**K1.00045** Electronic structure calculations for the fluctuating-bond model of high-temperature superconductivity, R. A. NISTOR, University of Western Ontario, D. M. NEWNS, C. C. TSUEI, G. J. MARTYNA, IBM T. J. Watson Research Center, M. H. MUSER, University of Western Ontario — High-temperature superconductors (HTS) have been intensely studied for the past 20 years due to their scientific and technological importance. The materials are characterized by square arrays of copper-oxygen-copper bonds. Although several salient features of HTS phenomena have been characterized, a working theory of the underlying physical processes in these materials has been lacking. Collaborators at IBM have recently proposed a model for HTS (Nature Physics 3, p. 184, 2007), involving a nonlinear coupling of the planar oxygen vibrations to the $d_{x^2−y^2}$ electrons on the copper. This interaction is modeled as a two-phonon coupling process in the resulting fluctuating-bond model (FBM). In the present work, we investigate the FBM theory by exploring the ability of the oxygens to buckle out of the straight Cu-O-Cu configuration by adjusting the charge on the copper atoms. The study is being conducted using Car-Parrinello simulations to investigate the electronic structure of the materials, and zero temperature single point DFT energy calculations to investigate the floppiness of the oxygen bonds. The aim is to justify, from first principles, the parameterization used in the FBM theory.

**K1.00046** Near-Zero Modes in Superconducting Graphene, POUYAN GHAEMI, FRANK WILCZEK, Massachusetts Institute of Technology — Vortices in the simplest superconducting state of graphene contain very low energy excitations, whose existence is connected to an index theorem that applies strictly to an approximate form of the relevant Bogoliubov-deGennes equations. When Zeeman interactions are taken into account, the zero modes required by the index theorem are (slightly) displaced. Thus the vortices acquire internal structure; the resulting “modicules” obey nonabelian quantum statistics.

**K1.00047** Do ‘magic’ Electronegativities exist for superconductivity?\(^3\) O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies[TCST], Abuja FCT, Nigeria — Studies have established a strong correlation between electronegativity and superconductivity. Here we examine the electronegativity values of many known binary superconducting systems[A15s, Y2C3, CaSi2, MgB2, ...] with high transition temperatures and use those[magic] values and their series to predict new superconducting materials. We also estimate the transition temperatures of the predicted compounds if they could be formed under pressure.

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\(^1\)This work was supported by NYSTAR grant.

\(^3\)With financial support from Mr. Ferguson Uzoma + Institute for Superconducting and Electronic Materials, University of Wollongong, NSW, Australia.
K1.00048 Bogoliubov angle and visualization of particle-hole mixture in1, ILYA GRIGORENKO, Los Alamos National Laboratory, KAZU FUJITA, JINHO LEE, ALFRED WANG, Cornell University, JIAN XIN ZHU, Los Alamos National Laboratory, J.C. DAVIS, Cornell University, HIROSHI EISAKI, Nanoelectronics Research Institute, AIST, Japan, S. UCHIDA, University of Tokyo, ALEXANDER BALATSKY, Los Alamos National Laboratory — Superconducting excitations — Bogoliubov quasiparticles — are the quantum mechanical mixture of negatively charged electron (−e) and positively charged hole (+e). Depending on the applied voltage bias in STM one can sample the particle and hole content of such a superconducting excitation. Recent Scanning Tunneling Microscope (STM) experiments offer a unique insight into the inner workings of the superconducting state of superconductors. We propose a new observable quantity for STM studies that is the manifestation of the particle-hole dualism of the quasiparticles. We call it a Bogoliubov angle. This angle measures the relative weight of particle and hole amplitude in the superconducting (Bogoliubov) quasiparticle. We argue that this quantity can be measured locally by comparing the ratio of tunneling currents at positive and negative biases. Bogoliubov angle allows one to visualize robustness of superconducting state locally. It may also allow one to measure the particle-hole admixture of excitations in normal state above critical temperature and thus to measure superconducting correlations in pseudogap state.

1Work supported by the BES and LDRD funds from U.S. Dept. of Energy at LANL under Contract No. DE-AC52-06NA25396 and from BNL under Contract No. DE-AC02-98CH18868.

K1.00049 ABSTRACT HAS BEEN MOVED TO SESSION W17 –

K1.00050 Electronegativity Spectrum Maps: A computational combinatorial materials synthesis and search tool, O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies (TCST), Abuja FCT, Nigeria — Using Pauling’s electronegativity scale of the elements from 0.7 to 4.0 we build a matrix of possible binary combinations in increments of 0.1 for binary systems _A_ _B_. We get a 34 x 34 spreadsheet of electronegativities. We call this an ElectroNegativity Spectrum Map (ENSMap). Each of the 1156 cells represents a possible combination of two electronegativities that could yield a binary compound. Using the correlation between electronegativity and superconductivity, we can identify from an ENSMap the electronegativities of known superconductors of a given binary class. We can also identify other electronegativity combinations that give the same electronegativity as a known superconductor. Here we show that ENSMAPS of binary systems can become a powerful computational combinatorial material synthesis tool and also a tool for searching for novel materials. We use ENSMaps to predict twenty new binary superconductors with high transition temperatures.

K1.00051 MAGNETISM (EXPERIMENT, THEORY, APPLICATIONS) –

K1.00052 Magnetic susceptibility and Mössbauer studies of [FeX_3](ClO_4)_2·H_2O with X = bpz, bpy, phen or ppy, J.C. HO, H.H. HAMDEH, R. KIRGAN, D.P. RILLEMA, Wichita State University — Magnetic studies have been made on several tris-chelated iron complex compounds [FeX_3](ClO_4)_2·H_2O with aromatic nitrogen heterocycle ligands X = bpz (2,2’-bipyrazine), bpy (2,2’-bipyridine), phen (1,10-phenanthroline) or ppy (2,2’,6,2’’-terpyridine). SQUID data (2-300 K and 0.01-1 T) yielded small effective magnetic moments, which are characteristic of low-spin Fe(II), in agreement with the isomer shift and quadrupole splitting values from Mössbauer measurements (4-300 K, 0-5 T). Meanwhile, apart from the expected diamagnetism, a positive term of temperature-independent paramagnetic susceptibility prevails in most cases.

K1.00053 Experimental Determination of Thermal Entanglement in Spin Clusters using Magnetic Susceptibility Measurements, R.S. SARTHOUR, A.M. SOUZA, Centro Brasileiro de Pesquisas Físicas, D.O. SOARES-PINTO, M.S. REIS, CICECO, Universidade de Aveiro, I.S. OLIVEIRA, Centro Brasileiro de Pesquisas Físicas — Until a few years ago, entanglement was not believed to exist beyond atomic scale, due to the large number of constituents of macroscopic objects. Surprisingly, it was theoretically demonstrated that entangled states can exist in solids at finite temperature. This phenomenon, referred to as “thermal entanglement”, is not an effect of the coupling between Mn-Mn ions, but it is a “universal” property of solids. Since then, a few experimental evidences have been confirmed reporting the presence of entanglement in solids state systems. The present work reports an experimental observation of thermal entanglement in a spin chain formed in the compound Na2CuSi3O14. The presence of entanglement was investigated through two measured quantities, an Entanglement Witness and the Entanglement of Formation, both derived from the magnetic susceptibility, determined experimentally. It was found that pairwise and tripartite entanglement exist below ~200 K and ~240 K, respectively. A theoretical study of entanglement evolution as a function of applied field and temperature is also presented.

K1.00054 Magnetic Structure and Magnetic Properties of CaMn2Sb2, A.L. LIMA SHARMA, Yeshiva University, A.M.S. GOMES, Universidade Federal do Rio de Janeiro, I.L. GONZALES, Pontificia Universidade Catolica do Rio de Janeiro — The AM2X2 ternary intermetallic (A = rare or alkaline earth, M = transition metal) compounds have revealed interesting magnetic properties due to the interplay between their magnetic sublattices. Pursuing the idea that the coupling between Mn-Mn ions can significantly affect electric transport properties, we investigated (Ca,Sr)Mn2Sb2 intermetallic compounds which presents two secondary magnetic transitions at 82K and 250K. Field dependent dc-magnetization curves for CaMn2Sb2 were obtained at two different temperatures, above and below 250K, show a relatively steep increase of the magnetization upon increasing the field to _H_ = 5 kOe, followed by a less steep and almost linear increase with the field and no tendency for saturation. The net macroscopic moment on the Mn at 300 K and 50 kOe is only a fraction of a Bohr magneton (ca. 0.15 _B_ / Mn), and evidently, a simple interpretation of its value in terms of localized high/low spin Mn_2+ _ions_ is unrealistic. The low moment can be viewed as a signature of the counterbalanced magnetic properties, which are dominated by the Eu-Eu superexchange coupling. The sharply defined Neel temperature increases with hydrostatic pressure ( _d_ _T_N_ / _d_ _P_ = +0.03 K/kbar at low pressures.)

K1.00055 Pressure Dependent Magnetism in Magnetically Ordered Interlanthanide Chalcogenides1, E.S. CHOI, Florida State University/NHMFL, R.P. GUERTIN, Tufts University, THOMAS ALBRECHT-SCHMITT, G.B. JIN, Auburn University — Several new interlanthanide chalcogenide compounds, Ln’/Ln”/Q (Ln’=light and Ln”=heavy lanthanide, Q=5 or Se) have been synthesized using a novel flux-growth technique, their complex structures determined, and their magnetic properties measured. The majority, with general formula Ln’Ln”Q_4_, are paramagnetic for _T_ > 2K, with effective moments consistent with the magnetic Ln constituents. Eu_2Ln_2Q_4_ (Ln’=Tb - Lu), which crystallize in the CaF_2O_4_-type three-dimensional channel structure, are all antiferromagnetic with _T_N_ ~ 3-5 K. The Ln constituent is geometrically frustrated and has secondary effects on the magnetic properties, which are obtained by the Eu-Eu superexchange coupling. The sharply defined Neel temperature increases with hydrostatic pressure to _P_~ 7 kbar for all EuLn_2Q_4_. (For example, for EuLu_2Se_4_, _dT_N_/dP = +0.03 K/kbar at low pressures.)

1Work supported by the US DOE through the EPSCoR program. NHMFL supported by NSF and the State of Florida.
K1.00056 Possible Exotic Magnetism in the Anti-Perovskite Nitride Cr$_3$PtN$^1$. J.R. THOMPSON, Univ Tennessee and Oak Ridge Natl Lab, M.P. BRADY, J.H. SCHNEIBEL, D.J. SINGH, E.A. PAYZANT, ORNL, J.W. SINCLAIR, A.P. SUBEDI, Univ Tennessee, A. MANIVANNAN, Natl Energy Tech Lab, M. SEEHRA, W VA Univ — Samples of the anti-Perovskite nitride Cr$_3$PtN were synthesized for bulk magnetism studies. X-ray diffraction confirmed the structure and several new phases within instrumental sensitivity ($\sim$-2.4 vol. %). Bulk magnetic properties were studied by SQUID magnetometry at $T = 5$-300 K in magnetic fields $H$ up to 6.5 T. Highly hysteretic ferromagnetism was found, with a Curie temperature $T_c \approx 110$ K. (Prior to nitriding, the Cr$_3$Pt starting material was paramagnetic.) At $5$ K, the coercive field $H_c$ is $\sim 2.3$ T. The curious and possibly exotic feature is that the saturation magnetic moment is small, 0.2 G-cm$^3$/gram: if the signal arises from bulk Cr$_3$PtN, the corresponding moment is only 0.1 $\mu_B$ per formula unit, which is quite small for a 100 K ferromagnetic. The saturation magnetization varies as $M_{sat} \sim (1/T)^{0.5}$ with critical exponent $\beta=0.40$. In isostuctural Pd-based Cr$_3$PtN (not single phase), no ferromagnetism was found above 5 K. DFT calculations of the band structure for the ideal anti-Perovskite compounds revealed a high electronic density of states $N(E_F)$ for Cr$_3$PtN and a somewhat lower value for Cr$_3$PdN.

$^1$Research sponsored by US DOE via the LDRP Program of ORNL.

K1.00057 Spin-reorientation transitions in Er, Tm and Yb orthoferrites: magnetic and structural properties. Y.A. BAZALIY, Leiden University, The Netherlands; University of South Carolina, Columbia, SC, USA; Institute of Magnetism, Kyiv, Ukraine, L. T. TSYMBAL, N. V. DERRKACHENKO, V. I. KAMENEV, O.Galkin Donets Physics and Technology Institute, National Academy of Science, Donets, Ukraine, G. N. KAKAZEI, Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain; Institute of Magnetism, National Academy of Science, Kyiv, Ukraine, F. J. PALOMARES, and Structural characteristics of ErFeO$_3$, TmFeO$_3$ and YbFeO$_3$ single crystals were studied over a wide temperature range. Magnetic measurements found that the spin-reorientation transitions in all crystals are well described by the earlier proposed theory with no fitting parameters. Additionally, they have shown the absence of the magnetic compensation point in TmFeO$_3$, and a noticeable growth of the c-axis magnetization at low temperatures in TmFeO$_3$ and ErFeO$_3$. The X-ray measurements found no symmetry-lowering lattice distortions during the reorientation. Overall, the measurements cover a wide range of material parameters and demonstrate the generality of the modified mean field theory of the $\Gamma_3 \rightarrow \Gamma_{24} \rightarrow \Gamma_2$ orientation phase transitions in orthoferrites. // L. T. Tsymbal et al., J. Appl. Phys 101, 123919 (2007).

K1.00058 Magnetostatic Interactions in Partially Shielded Polyaniline-Ferromagnet Composite Nanowire Arrays. ADAM FRIEDMAN, DERRICK BRITTAIN, LATIKA MENON, Northeastern University Dept. of Physics — Ferromagnetic nanowires have remarkable magnetic properties including high coercivities and strong magnetic shape anisotropy. These unique properties have been theoretically studied and various models attribute the observed characteristics to inter- and intra-wire magnetostatic interactions, which are a function of the structure of the nanowires and their coupling with the applied magnetic field. In this study, we use porous alumina templates and electrodeposition to fabricate Fe, Ni, and Co nanowires, creating magnetically shielded ferromagnet structures. We measure the magnetic properties of these structures as a function of their diameter and temperature in order to better understand the magnetic interactions that arise in ferromagnetic nanowire arrays. By partially shielding the wires with PAni, we are able to better discern the effects of these interactions. Results will be presented and compared to theoretical models.

K1.00059 Dipolar effect in the standing spin waves of dot structures$^1$. C. YU, M. PECHAN, Department of Physics, Miami University of Ohio — Standing spin waves in dot structures are generally described by dipole-exchange mechanisms. In this work, the role of dipolar coupling has been probed via micromagnetic simulation of spin wave mode structure on a circular, permalloy dot, 200nm diameter, 40nm thickness containing a concentric gap (ring) void of magnetic material. This gap precludes exchange coupling between the inner dot and the outer ring of the overall ferromagnet structures. We measure the magnetic properties of these structures as a function of their diameter and temperature in order to better understand the magnetic interactions that arise in ferromagnetic nanowire arrays. By partially shielding the wires with PAni, we are able to better discern the effects of these interactions. Results will be presented and compared to theoretical models.

$^1$Acknowledgement: This work is supported by U.S. DoE at MU and U.S ONR-MURI at UM.

K1.00060 Absence of Hole Confinement in Transition Metal Oxides with Orbital Degeneracy$^3$. MARIA DAGOHER, University of Tennessee, KRZYSZTOF WOHLFELD, ANDRZEJ M. OLES, Jagiellonian University, ENRICO ARRIGONI, Graz University of Technology, PETER HORSCH, Max-Planck-Institut FKF — The compounds with orbital degrees of freedom exhibit many possible scenarios for hole propagation which in most cases lead to hole localization [1]. Here we investigate the spectral properties of a hole moving in a two-dimensional Hubbard model for strongly correlated $t_{2g}$ electrons. Although superexchange interactions are Ising-like, a quasi-one-dimensional coherent hole motion arises due to effective three-site terms. This mechanism is fundamentally different either from the hole motion via quantum fluctuations in the conventional spin model with SU(2) symmetry or from the $e_g$ orbital model [2]. The present orbital model describes also propagation of a hole in some $e_g$ compounds [3], and we argue that orbital degeneracy alone does not lead to hole self-localization. [1] J. Zaanen and A.M. Oleś, Phys. Rev. B 48, 7197 (1993). [2] J. van den Brink, P. Horsch, and A.M. Oleś, Phys. Rev. Lett. 85, 5174 (2000). [3] M. Daghofer, A.M. Oleś, and W. von der Linden, Phys. Rev. B 70, 184430 (2004).

$^3$We acknowledge support by Foundation for Polish Science (FNP), by the Polish Ministry of Science and Education Project No. N202 068 32/1481, and by the Austrian Science Fund (FWF Project P18505-N16).

K1.00061 Magnetic phase separation in LaMn$_{1-x}$Fe$_x$O$_{3+y}$, O.F. DE LIMA, Instituto de Fisica Gleb Wataghin, UNICAMP, Campinas, J.A.H. COAQUIRA, R.L. DE ALMEIDA, J.B. DE CARVALHO, S.K. MALIK, Centro Internacional de Fisica da Materia Condensada, UnB, Brasilia — We have investigated the LaMn$_{1-y}$Fe$_y$O$_{3+y}$ system in the whole composition range 0$\leq y \leq 1$, for polycrystalline samples prepared by solid state reaction in air. All samples show orthorhombic structure (space group Pnma). For $x=0$ the oxygen excess, estimated to be $y \approx 0.1$, produces vacancies in the La and Mn sites and generates a fraction around 20% of Mn$^{4+}$ ions (3t$_2g$) and 80% of the usual Mn$^{3+}$ ions (3t$_2g$, 1e$_g$), with possible double exchange interaction between them. The Fe-doping in this system is known to produce only stable Fe$^{3+}$ ions (3t$_2g$, 2e$_g$). We find an evolution from a fairly strong ferromagnetic (FM) behavior, with saturation magnetization (T=2K) $m_S \approx 4 \mu_B$ and Curie temperature $T_C \approx 160$ K, for $x=0$, to an antiferromagnetic (AFM) behavior, with $T_N=790$ K, for $x=1$. For intermediate Fe contents a mixed phase scenario occurs, with a gradual decrease (increase) of the FM (AFM) phase, accompanied by a systematic transition broadening for 0.2$<x<0.7$. A calculation based on the expected exchange interaction among the various magnetic-ion types, accounts very well for the $m_S$ dependence on Fe doping.

$^3$We acknowledge the Brazilian agencies FAPESP, CNPq and CAPES.
K1.00062 The Friedel-Anderson Impurity with Orbital Degeneracy. LIYE ZHANG, GERD BERGMANN, Univ. of Southern California — A recently developed compact solution for the non-degenerate Friedel-Anderson impurity is extended to impurities with orbital degeneracy. The singlet ground state is investigated for two and three orbits (corresponding to four and six d-states). The ground state energy and the multi-d-state occupations are calculated. The magnetic moment (above the Kondo temperature) is obtained in different regions of the parameter space of $V_{dd}$ (s-d-hopping matrix element), $E_g$ (d-state energy), $U$ and $U_d$ (Coulomb and exchange energies). The average d-state occupation can be adjusted to about one, two or three d-electrons. A comparison between different orbital degeneracy but the same d-state occupation is performed. The role of the Coulomb and the exchange interaction in the magnetic and singlet states is analyzed. The challenges for the treatment of a real d-impurity with five d-orbits is discussed.

K1.00063 Magnetic and charge correlations in the frustrated 2D Hubbard model1. MATTHEW ENJALRAN, Department of Physics, Southern CT State University, 501 Crescent St., New Haven, CT 06515 — The high temperature superconductors have motivated numerous theoretical studies of strongly correlated many-body systems for over two decades. The richness of the phase diagram of these materials belies their relatively simple quasi-two-dimensional structure of stacked CuO$_2$ planes, where copper ions form a square lattice. With the experimental observation of several complex phases, including superconductivity, in quasi-two-dimensional triangular lattice materials (e.g., Na$_x$CoO$_2$, $\delta$H$_2$O and $\kappa$-(ET)$_2$X) we now have material systems in which geometric frustration plays a prominent role. With this as our motivation, we investigate the 2D Hubbard model on a series of lattice geometries. The results show some interesting tendency towards new phases for the frustrated systems. We conclude with a discussion of the potential application of the constrained path quantum Monte Carlo (CPQMC) method to the study of frustrated 2D Fermi systems.

*K1.00064 Identification of Bosonic Mode in the Electron-Doped Superconductor Pr$_{1.05}$LaCu$_{12}$O$_{29.5}$, SHANKAR KUNWAR, FRANCIS NIESTEMSKI, SEN ZHOU, Department of Physics, Boston College, Chestnut Hill, MA, 02467, SHILIANG LEE, University of Tennessee, Knoxville, TN, 37996, HONG DING, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA, 02467, PENGCHENG DAI, University of Tennessee, Knoxville, TN, 37996, MADHAVAN VIDYA, Department of Physics, Boston College, Chestnut Hill, MA, 02467 — It is well known that in the superconducting state, the current carriers are the cooper pairs, where two electrons (fermions) get paired up by a mediator (glue) and behave as a single boson. In conventional superconductors, lattice vibrations (phonons) act as a glue to pair up the electrons, however, in high T$_c$ superconductors, the mechanism that binds these fermions together is still unclear. There are two principal contenders for the glue: phonons and the spin excitations. Using high resolution STM we have probed an electron-doped superconductor, Pr$_{1.05}$LaCu$_{12}$O$_{29.5}$, and identified a bosonic excitation at 10.5 ± 2 meV which could potentially act as the superconducting glue. The energy scale of this mode rules out an explanation in terms of the oxygen optical phonons confining the possibilities to spin excitations and the acoustic phonons. This finding potentially takes us one step closer to identifying the superconducting glue in High T$_c$ superconductors.

K1.00065 Investigating the Structure of La$_2$CuGa$_{12}$, Using Neutron Powder Diffraction. JASMINE MILLICAN, National Institute of Standards and Technology, JUNG YOUNG CHO, JULIA CHAN, Louisiana State University, JUDITH STALICK, National Institute of Standards and Technology — Single crystals of a new phase, La$_2$CuGa$_{12}$, have been synthesized using flux growth. Preliminary single crystal X-ray diffraction results suggest La$_2$CuGa$_{12}$ to be isostructural to Ce$_2$PdGa$_{12}$ and crystallize in the P$4$/nmb space group with lattice parameters of $a$ ~ 6.179 Å and $c$ ~ 15.384 Å. Residual electron density, which was observed in the Fourier difference map of the single crystal X-ray diffraction data, and the observation of satellite peaks in the data are indicative of the possibility of statistical disorder in La$_2$CuGa$_{12}$. In addition, unusual behavior of thermal parameters for an additional Ga position is observed in the X-ray diffraction data of La$_2$CuGa$_{12}$. Although a preliminary model has been constructed using single crystal X-ray diffraction experiments, due to the two electron difference between $^{67}$Ga and $^{61}$Ga, neutron powder diffraction experiments may be a more suitable probe in accurately determining the structure and site occupancy of the additional Ga atom in La$_2$CuGa$_{12}$. We have employed neutron powder diffraction (BT-1) to investigate the structure in the phase, La$_2$CuGa$_{12}$.

K1.00066 Synthesis and Characterization of High Quality Single Crystal CeCoIn$_5$, ABEBE KEBEDE. TERREL DIAL, NC A&T State University — The preliminary results on the structure and electronic properties of (Re, Ce)(Co, M)In$_5$ are presented. Here R = Pr and M = Fe. We present the results of our measurements of resistivity, specific heat and magnetization. This work is supported by the Department of Energy Grant # DE-F052-05NA27036.

K1.00067 Spin valve electrode for organic light emitting devices. LIANBIN NIU, YUNXIA GUAN, YUE REN, CHUNYANG KONG, YAN MA, YIPEING LIAN, YAN FANG, Department of Physics, Chongqing Normal University — Effects of spin filter on singlet and triplet exciton fractions in organic light-emitting devices (OLEDs) is attracting considerable attention nowadays. Electroluminescence in organic semiconductors strongly depends on the relative population of singlet and triplet excitonic states. Controlling the spin statistics by injecting and transporting carriers with defined spin orientation can amplify a chosen electronic transition increasing the device efficiency or changing the emission spectral band. A spin valve was used as hole injector, substituting the traditional indium tin oxide electrode. A comparison of electroluminescence and IV curves between similar devices with and without spin valve electrode is reported. The result shows that spin valve can successfully replace conventional electrode in OLEDs.

K1.00068 Nonlinear current-voltage characteristics of oxygen-deficient La$_{0.67}$Ca$_{0.33}$MnO$_{3-y}$ films1. SHIU-JEN LIU, Department of Materials Engineering, Mingchi University of Technology, J.Y. JUANG, Department of Electrophysics, National Chiao Tung University, J.Y. LIN, Institute of Physics, National Chiao Tung University, K.H. WU, T.M. UEN, Department of Electrophysics, National Chiao Tung University, Y.S. GOU, Department of Physics, National Taiwan Normal University — Two different types of nonlinear current-voltage characteristics are observed in oxygen-deficient La$_{0.67}$Ca$_{0.33}$MnO$_{3-y}$ (LCMO) films at temperatures below insulator-metal transition. The parabolic-like dynamic conductance $G(V)$, defined as $dI/dV$, curves near zero bias observed in highly oxygen-deficient LCMO films implies the contribution from the spin-dependent tunneling transport between ferromagnetic clusters with magnetic-disordered regions serving as tunneling barriers. On the other hand, for the slightly oxygen-deficient LCMO films, dips around zero bias were observed in nonlinear $G(V)$ curves and have been attributed to spin-flip scattering with oxygen vacancies serving as scattering centers.

1Supported by the National Science Council of Taiwan, under Grant No. NSC 95-2112-M-131-002-MY3
K1.00069 Anisotropies in Quaternary Intermetallic Compounds, W.C. LEE, Dept. of Physics, Sookmyung Women's Univ. Seoul 140-742, Korea — From the high-temperature series expansion of magnetic susceptibilities and the anisotropic Weiss temperatures, the first Stevens' parameter, $B_2^0$, and the magnetic exchange interaction constant $J_{1x}$ of each $R^3$ ions magnetic sublattice in quaternary intermetallic compounds, $R_{1}R_{2}B_{x}C_{y}(R=R_{tm}, R_{h}, D_{y}, T_{b})$ were obtained. The $R= Dy$ system shows the biggest $B_2^0$ value and the $R= Tb$ system does the smallest one. Also we have applied the anisotropic M(H) isotermers as a function of applied magnetic fields for H perpendicular and parallel to the c-axis for each compounds to check out our crystalline electric field (CEF) results obtained from the previous mentioned method by using the anisotropic Weiss temperatures. It turned out that most of the temperature dependence of magnetization curve M (T) for H perpendicular the c-axis at low temperature comes from the temperature dependent population of the singlet ground state in group L among groups L(low-lying levels of ground states), H(high levels of ground states), and M(first excited states).

K1.00070 Anisotropy in the magnetodielectric constant in orthorhombic HoMnO$_3$ thin film, SUNG HO LEE, BONG YEOL LEE, MIN HWAX JUNG, YOON HEE JONG, Pohang University of Science and Technology, Pohang, Korea — Epitaxial HoMnO$_3$ thin films in the metastable orthorhombic structure were successfully synthesized on SrTiO$_3$ substrates by pulsed laser deposition. The crystal structure, surface roughness, and surface morphology of the films were characterized by various tools such as X-ray diffraction, atomic force microscopy, scanning electron microscopy etc. Macroscopic physical properties were measured with a Quantum Design PPMS. It is found that an significant increase of the dielectric constant accompanies the onset of magnetic order at 45 K in the films. This then proves that there exists a magnetodielectric coupling in orthorhombic HoMnO$_3$. Anisotropy in the magnetodielectric constant was observed according to the direction for an external magnetic field. These behaviors will be compared to the cases of YmMnO$_3$ and BiMnO$_3$. Measurements of the reverse effect, that is, the variation of the magnetic susceptibility with an electric field, are being attempted.

K1.00071 ABSTRACT WITHDRAWN

K1.00072 Diffraction-induced magneto-optical enhancement in gyrotropic gratings, YUEHUI LU, MINHYUNG CHO, JINBAE KIM, GEONJOON LEE, YOUNGPAK LEE, q-Psi and BK21 Program Division of Advanced Research and Education in Physics, Hanyang University, Seoul, Korea, — The spectra of diffrekted magneto-optical Kerr effect (D-MOKE), for polar magnetization in one-dimensional gyrotropic gratings, were presented by Antos et al. [Appl. Phys. Lett. 86, 231101 (2005)]. It was noted that the magnitude of Kerr rotation in the first-order diffraction was one order higher than that of the zeroth-order diffraction in most of the energy range. In this study, a rigorous coupled-wave approach, implemented as Airy-like internal series, was applied to investigate the diffraction-induced MO enhancement. The simulated spectra of D-MOKE are consistent with their experimental ones. Moreover, it was found that the magnitude ratio of the first-order Kerr rotation to the zeroth-order one was strongly dependent on the grating depth. In other words, D-MOKE can be effectively modulated by the groove depth. This theoretical approach is of great significance in designing and applying the diffracted MO elements.

K1.00073 Synthesis and magnetic properties of Zn$_{1-x}$Mn$_x$O/ZnO coaxial nanocable, D. WANG, S. PARK, Y. LEE, T. EOM, Y. LEE, q-Psi and BK21 Program Division of Advanced Research and Education in Physics, Hanyang University, Seoul, Korea — Zn$_{1-x}$Mn$_x$O/ZnO ($x=0.04$ and 0.20) coaxial nanocables were prepared by using an ultrahigh-vacuum radio-frequency magnetron sputtering system. The samples were characterized by scanning electron microscopy (SEM), x-ray diffraction (XRD), Rutherford backscattering and high-resolution transmission electron microscopy (HR-TEM), and with a superconducting quantum interference device magnetometer. The SEM images show that the morphology and the alignment of ZnO nanocables are maintained after the deposition of Zn$_{1-x}$Mn$_x$O layer, and the thickness of Zn$_{1-x}$Mn$_x$O layer is about 20 nm. The XRD analysis reveals that Mn is incorporated well into the wurtzite ZnO without forming Mn oxide. The HR-TEM image shows that both ZnO core layer and Zn$_{1-x}$Mn$_x$O shell layer are single crystalline and an excellent epitaxial growth has been achieved. The magnetic property measurement indicates that the Zn$_{0.96}$Mn$_{0.04}$/ZnO coaxial nanocable is in the ferromagnetic state at 300 K as well as at 10 K, while Zn$_{0.80}$Mn$_{0.20}$/ZnO is nonferromagnetic even at 10 K and the bare ZnO nanorod is diamagnetic. The aging effect of the magnetics for Zn$_{0.96}$Mn$_{0.04}$/ZnO coaxial nanocable was also investigated, and it was found that the aged sample showed a mixed magnetic phase of ferromagnetism and paramagnetism.

K1.00074 Enhanced magneto-optical effect in one-dimensional spin photonic crystals, J.B. KIM, J.Y. RHEE, BK21 Physics Research Division and Institute of Basic Sciences, Sungkyunkwan University, Suwon, Korea — Spin photonic crystals (SPCs) are very interesting for information technology which requires advanced solutions for heavy communication traffic, high-density storage, and high-speed computing. By using external magnetic field, for instance, the optical properties of SPCs can be tuned. By using the interference pattern of two femtosecond-laser beams, a selective-area annealing of the as-deposited Co$_2$Mn$_2$Si film was achieved and one-dimensional SPCs were fabricated. The atomic-force-microscopy results confirmed that regularly spaced alternating lines with a periodicity of 2 μm were produced, and the magnetic-force-microscopy studies revealed the same periodic patterns of magnetic domains. The longitudinal Kerr rotations of the p-polarized zeroth-order and first-order diffracted beams were measured. The longitudinal Kerr rotation of the first-order diffracted beam turns out to be nearly 28 times larger with respect to the zeroth-order one.

K1.00075 Size dependent magnetic properties of magnetite (Fe$_3$O$_4$) nanoparticles, SONGJIN JANG, SAVAS DELIKANLI, HAO ZENG, University at Buffalo-SUNY — Magnetism of magnetite (Fe$_3$O$_4$) nanoparticles was studied as a function of the particle size. Fe$_3$O$_4$ nanoparticles with different size from 3 nm to 10 nm were synthesized by high temperature organic solution phase method. Hysteresis loops of all the particles showed superparamagnetic behavior at room temperature. The blocking temperature ($T_B$) decreases with decreasing particle size. All hysteresis loops were fitted by the Langevin's function, where the saturation magnetization ($M_s$) was extracted. $M_s$ was further deduced by using the saturated moment and accurately measured mass of the particles. The two methods agree with each other excellently. $M_s$ decreases as the particle size is decreased, and is in general much smaller than that of bulk. $M_s$ shows a sharp drop with increasing temperature at low temperatures and deviates from the $T^{3/2}$-law. This behavior is attributed to competing ferromagnetic and antiferromagnetic exchange interactions which contribute differently at the surface and interior of the particles.

1Work supported by NSF DMR 0547036.

K1.00076 Ab initio study of the possibility of noncollinear magnetism in small Mn clusters, R.C. LONGO, MANUEL ALEMANY, Universidad de Santiago de Compostela, Spain, J. FERRER, Universidad de Oviedo, Spain, A. VEGA, Universidad de Valladolid, Spain, L. J. GALLEGO, Universidad de Santiago de Compostela, Spain — We investigated the possibility of noncollinear magnetism in small Mn$_n$ clusters ($n=2-6$) using the density-functional method SIESTA with the generalized gradient approximation (GGA) to exchange and correlation. The lowest-energy states identified were ferromagnetic for Mn$_2$ and Mn$_4$, and magnetically noncollinear for Mn$_3$, Mn$_5$, and most decidedly, Mn$_6$. These SIESTA/GGA results, which are compared with those of an earlier SIESTA study that used the local spin density approximation, are qualitatively in keeping with the result obtained by VASP/GGA calculations.

1Work supported by the Spanish Ministry of Education and Science (Projects FIS2005-04239, FIS2006-12117-C04-04, MAT2005-03415 and Program “Ramon y Cajal”), by the Junta de Castilla y Leon (Grant No.VA068A06), and by the Galician Supercomputing Center.
K1.0077 Microscopic simulation and a spin crossover transition. HAROLD O. JESCHKE, L. ANDREA SALGUERO, ROGER VALENTI, Institut fuer Theoretische Physik, Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany. BADIUR RAHMAN, TANUSRI SAHA-DASGUPTA, S.N. Bose National Centre for Basic Sciences, JD Block, Sector 3, Salt Lake City, Kolkata 700098, India, CHRISTIAN BUCHBAUM, VOLODYMIR PASHCHENKO, MARTIN U. SCHMIDT, Institut fuer Anorganische und Analytische Chemie, Universitaet Frankfurt, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany. — In spin crossover materials, an abrupt phase transition between a low spin state and a high spin state can be driven by temperature, pressure or illumination. Of a special relevance are Fe(II) based coordination polymers where, in contrast to molecular systems, the phase transition shows a pronounced hysteresis which is desirable for technical applications. A satisfactory microscopic explanation of this large cooperative phenomenon has been sought for a long time. The lack of X-ray data has been one of the reasons for the absence of microscopic studies. In this work, we present an efficient route to prepare reliable model structures and within ab initio density functional theory analysis and effective model considerations we show that in polymeric spin crossover compounds magnetic crossover effects between high spin Fe(II) centres is as important as elastic couplings for explaining the considerable cooperativity and thus the width of the hysteresis.

K1.0078 Statistical mechanics and thermodynamics in anisotropic Heisenberg-like nanoclusters. ARMEN KOCHARIAN, Department of Physics and Astronomy, California State University, LEV ANANIKYAN, SERGEI POGHOSYAN, NERSES ANANIKYAN, Varennes Physics Institute. The single magnetic excitations thermal entanglements in nanoclusters are compared to the points are studied in small spin s = 1/2 and 1 in ferromagnetic and antiferromagnetic Heisenberg clusters. The grand canonical ensemble of Heisenberg clusters is also used for exact calculations of thermal properties, quantum and thermal entanglements of the spin lattice models in the presence of magnetic field and anisotropic field. We study the magnetic phase transitions and crossovers in clusters of various topologies driven by exchange interaction, external field and temperature. The comparison with the exact solution for the Heisenberg model in thermodynamic limit for the limiting cases is also provided. The small Ising and Heisenberg clusters are also used for comparison with the exact Bethe-ansatz solutions. These exact results in clusters give a novel insight into the properties of single molecule magnets, the dynamics of magnetization and can be useful for interpretation of the phase diagram in molecular nanomagnets and nanometer-sized magnetic particles. 

K1.0079 muSR in Ba$_2$CoO$_4$, PETER RUSSO, TRIUMF, JUN SUGIYAMA, Toyota CRDL, EDUARDO ANSALDO, TRIUMF, JESS BREWER, SCOTT STUBBS, UBC, KIM CHOW, University of Alberta, R. JIN, Oak Ridge, H. SHA, J. ZHANG, Florida International University. — A positive muon spin rotation and relaxation ($\mu$SR) experiment on the single crystal Ba$_2$CoO$_4$ indicates the existence of an antiferromagnetic (AF) transition occurring at $T_N$ $\sim$25 K. Weak transverse field measurements ($\mu$TF-$\mu$SR) show that the paramagnetic volume fraction of the sample decreases rapidly at the magnetic transition indicating a bulk effect. Zero field measurements (ZF-$\mu$SR) show the presence of a magnetically ordered state below $T_N$. The results are compared to recent magnetic susceptibility and neutron measurements. Although there are two possible AF spin structures proposed by recent neutron experiments, the $\mu$SR results clearly exclude AF order along the $c$-axis while supporting AF order in the ab plane.

K1.0080 Inelastic Neutron Scattering Excitations for a Spin $\frac{3}{2}$ Tetramer: Application to Magnetic Excitations in Na$_2$RuO$_4$. J. T. HARALDSEN, University of Tennessee, M.B. STONE, M.D. LUMSDEN, Oak Ridge National Laboratory, T. BARNES, University of Tennessee/Oak Ridge National Laboratory, R. JIN, Oak Ridge National Laboratory. — In an effort to explain the magnetic properties of such low-dimensional systems, $^{87}$Rb Nuclear Magnetic Resonance (NMR) experiments in a Na$_2$RbCu$_4$(AsO$_4$)$_2$Cl$_2$ system were performed. This novel two-dimensional (2D) cuprate contains layers of coupled CuO$_4$ tetramers. The spin exchange interactions are confined to 2D layers and the Cu are divalent, making the system an anisotropic, non-collinear AFM. In zero applied magnetic field, it orders antiferromagnetically via a second-order phase transition at $T_N$=15(1) K. The ordered state was characterized by $^{87}$Rb NMR, and a non-collinear rather than collinear arrangement of spins was suggested. New structural phase transition(s) around 74 and 110 K were also evidenced. We present a $\mu$SR study of this cuprate. The investigation of the spin dynamics (via the muon longitudinal relaxation rate $\lambda(T)$) in the temperature range 2<T<300K in zero-field, with particular attention to the order parameter below $T_N$ and around structural phase transitions at T$\sim$74K and T$\sim$110K is presented.

K1.0081 $\mu$SR study of spin dynamics and phase transition of the two-dimensional tetramer-cuprate Na$_2$RbCu$_4$AsO$_4$Cl$_2$. ANNAKI KRIISA, RAIVO STERN, National Institute of Chemical Physics and Biophysics, SHIOU-JHY HWU, WENDY QUEEN, Department of Chemistry, Clemson University, HUBERTUS LUETKENS, Laboratory for Muon-Spin Spectroscopy Paul Scherrer Institut — In an effort to explain the magnetic properties of such low-dimensional systems, $^{87}$Rb Nuclear Magnetic Resonance (NMR) experiments in a Na$_2$RbCu$_4$(AsO$_4$)$_2$Cl$_2$ system were performed. This novel two-dimensional (2D) cuprate contains layers of coupled CuO$_4$ tetramers. The spin exchange interactions are confined to 2D layers and the Cu are divalent, making the system an anisotropic, non-collinear AFM. In zero applied magnetic field, it orders antiferromagnetically via a second-order phase transition at $T_N$=15(1) K. The ordered state was characterized by $^{87}$Rb NMR, and a non-collinear rather than collinear arrangement of spins was suggested. New structural phase transition(s) around 74 and 110 K were also evidenced. We present a $\mu$SR study of this cuprate. The investigation of the spin dynamics (via the muon longitudinal relaxation rate $\lambda(T)$) in the temperature range 2<T<300K in zero-field, with particular attention to the order parameter below $T_N$ and around structural phase transitions at T$\sim$74K and T$\sim$110K is presented.

K1.0082 Spin dynamics of La$_{0.845}$Sr$_{0.155}$Mn$_{1-x}$M$_x$O$_3$ (M = Mn, Cu, Co) perovskites. MANH-HUONG PHAN, HARIHARAN SRIKANTH, University of South Florida, Tampa, FL 33620, THE-LONG PHAN, Micro- and Nano-Structures Group, H. H. W. Physics Lab, University of Bristol, Bristol BS8 1TL, UK. — Influence of the spin-lattice coupling on the magnetoresistance and magnetocaloric properties of La$_{0.845}$Sr$_{0.155}$Mn$_{1-x}$M$_x$O$_3$ (M = Cu, Co) perovskites has been investigated by means of electron spin resonance (ESR) spectroscopy. It was observed that asymmetrical ESR signals due to ferromagnetic correlations at temperatures T $<$ $T_{max}$, became Lorentzian at T $>$ $T_{max}$, where $T_{max}$, corresponds to the narrowest ESR linewidth. The temperature dependence of the ESR intensity, I(T), for the samples was well described by an expression of I(T) = I$_{0}$ $\exp$(E$_{g}$/k$_{B}$T). In the high temperature region, I(T) obeyed the Curie-Weiss law. The minimum linewidth, $\Delta$H$_{min}$, was determined to be 674, 890 and 750 Oe for La$_{0.845}$Sr$_{0.155}$Mn$_{0.98}$Co$_{0.02}$O$_3$ and La$_{0.845}$Sr$_{0.155}$Mn$_{0.98}$Cu$_{0.02}$O$_3$, respectively. This indicated an improvement of the spin-lattice coupling in samples with Cu or Co addition. The strongest spin-lattice coupling resulted in the largest magnetocaloric effect in La$_{0.845}$Sr$_{0.155}$Mn$_{0.98}$Cu$_{0.02}$O$_3$. The addition of Cu or Co in La$_{0.845}$Sr$_{0.155}$Mn$_{0.98}$O$_3$ reduced its ferromagnetism and conductivity. The mechanism of the spin-lattice coupling is discussed.

K1.0083 Competition between magnetic structures in the Fe-rich fcc FeNi alloys. IGOR ABRIKOSOV, ANDREAS KISSAVOS, FRANCOIS LIOT, BJORN ALLING, SERGEI SIMAK, Department of Physics, Chemistry and Biology, Linkoping University, Sweden, OLEG PEIL, ANDREI RUBAN, Applied Materials Physics, Royal Institute of Technology, Sweden. — We report on the results of a systematic ab initio study of the magnetic structure of Fe rich fcc FeNi binary alloys for Ni concentrations up to 50 at. %. Calculations are carried out within density functional theory using two complementary techniques, one based on the Exact Muffin-Tin Orbital theory within the coherent potential approximation and another one based on the Projector Augmented-Wave method. We observe that the evolution of the magnetic structure of the alloy with increasing Ni concentration is determined by a competition between a large number of magnetic states, collinear as well as non-collinear, all close in energy. We emphasize a series of transitions between these magnetic structures, in particular we have investigated a competition between disordered local moment configurations, spin spiral states, the double layer antiferromagnetic state, and the ferromagnetic phase, with a single spin flipped with respect to all others. We show that the latter should be particularly important for the understanding of the magnetic structure of the Invar alloys.
K1.00084 One-Dimensional Magnetic Chain Fragmentation in Ti/Ga Modified Multiferroic DyMn$_2$O$_5$. SUN-HEE KANG, HAI-JOON LEE, ILL-WON KIM, University of Ulsan, TAE-HWAN JANG, YOON-HEE JEONG, Pohang University of Science and Technology, TAE-YEONG KOO, Pohang Accelerator Laboratory, Pohang University of Science and Technology — We have studied the effect of Ga$^{3+}$ substitution into Mn$^{3+}$ site in DyMn$_2$O$_5$ on its multiferroic characteristics. Crystallographic structural, thermal, dielectric and magnetic properties are measured and discussed in terms of the dilution of magnetic Mn$^{3+}$ ions. Replacement of Mn$^{3+}$ ions with Ga$^{3+}$ changes the compound into a disordered multiferroic system and colossal magnetoelectric effect observed in DyMn$_2$O$_5$ disappears quickly below x<0.1 in DyMn$_{1-x}$Ga$_x$O$_5$. However as the content of Ga increases above x>0.1, a new type of ferroelectric transition identified by a peak in dielectric constant is evolved from the slowly varying dielectric background. Moreover remarkable enhancement of dielectric constant at ferroelectric transition temperature is continued even up to the solubility limit of Ga (x=0.2). This observation suggests a possible example of the channel for ferroelectricity in the disordered multiferroic system.

K1.00085 Maser Generation of Hypersound From Heat Through Adiabatic Demagnetization of a Paramagnetic Crystal. MICHAEL VAISFEL'D, Kingsborough College of CUNY — It has been shown in our earlier work on thermal masers [Sov. Phys. - JETP (USA), v. 57, No. 6, pg. 1263-9 (1983)] that the energy of thermal phonons of a crystal like La$_2$Mg$_3$(NO$_3$)$_2$·24H$_2$O (LaMN) doped with $^{16}$CO$^{3+}$ (ions A) and Ce$^{3+}$ (ions B) can be converted directly into the energy of coherent microwave radiation. Maser action has been observed at liquid helium temperatures in the 0.18-T static magnetic field after termination of the 1-T magnetic field pulse (which is applied for the adiabatic cooling of the electron spins 1/2 of the ions B). A partial population inversion is achieved in the system of hyperfine magnetic spin sublevels of the ions A as a result of the fast resonant thermal mixing between the nuclear spins I = 7/2 of the ions A and the cooled spins B. Our device acts as a quantum heat engine, without any microwave or optical pumping. Here we propose an analogous easily tunable pulsed phonon maser. The laser crystals of KY(WO$_4$)$_2$ [Eur. Phys. J. B 55, 388-395 (2007)] doped with $^{16}$E$^{3+}$ and $^{17}$I$^{3+}$ (I = 1/2) or $^{137}$I$^{3+}$ (I = 5/2) ions are proposed as working substances (instead of the crystal hydrate of LaMN:Ce$^{3+}$; $^{50}$Co$^{2+}$).

K1.00086 Magnetic and Structural Properties of Magnetite in Radicular Teeth of Chiton Acanthochiton Rubrolinestus. Y.N. HAN, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, C.L. LIU, College of Chemistry-biology Science & Technology, YanTai University, Shandong 264005, China, L.D. YAO, Y. WANG, X.F. HAN, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China — The major radular lateral teeth of Polyplacophora Chiton comprise a magnetic biomimetic cap. We have investigated the structure and magnetic properties of the biomimarized magnetite crystalites in mature teeth of Chiton Acanthochiton Rubrolinestus. From the measurement of magnetic properties of tooth particles using SQUID magnetometry we find that the saturation magnetization and the Verwey transition temperature ($T_v$) are 78.4 emu/g and 105 K, respectively. An in situ examination of the structure of magnetite-bearing region within individual tooth using the high resolution TEM, together with electron diffraction (ED) pattern and energy-dispersive X-ray (EDX) analyses indicates magnetite microcrystal form electron-dense polycrystalline sheets with typical length 800 nm and width 150 nm or so. These polycrystalline sheets are arranged regularly along the longitude direction of the tooth cutting surface. Furthermore, the microcrystallites in polycrystalline sheet take on the generally good crystallinity.

K1.00087 Heat diffusion in a classical Heisenberg chain. GONZALO GUTIERREZ, University of Chile, Chile. EDUARDO VALDEBENITO, University of Chile, SERGIO DAVIS, Royal Institute of Technology, Sweden — We study the heat transport in a one dimensional classical Heisenberg chain by means of spin dynamics simulation. The system consists of a $N=2000$ spins in the microcanonical ensemble, and the temperature is evaluated using the so-called configurational temperature formula. We thermalize the system to an equilibrium state at low temperature, and then we give a delta function energy packet in the middle of the chain. Studying both qualitatively and quantitatively the spreading of the delta, we characterize the diffusion of heat in the chain. In fact, calculating the second moment of the pulse, and using the relation

$$\langle \sigma(t)^2 \rangle = 2D\alpha^2, \quad (0 < \alpha < 2),$$

where $\sigma$ is the width of the pulse, $D$ is the diffusion constant and $\alpha$ is a parameter which consider the kind of diffusion. According our simulation, the heat in this system transports subdiffusively. This result imply that the system becomes a thermal insulator in the thermodynamic limit $N \rightarrow \infty$.

1) Grant Anillo ACT/24-Chile.

K1.00088 Magnetic properties of a mechanically alloyed metastable Cu$_{1-x}$Co$_x$ system. P. PRIETO, Excellence Center for Novel Materials, CENM, Cali - Colombia. D. REYES, A. CORTES, M. E. GOMEZ, W. LOPERA, Thin Film Group, Department of Physics, Universidad del Valle, AA. 25360, Cali - Colombia, M. LOPEZ, Departamento Ing. de Materiales, Universidad de Concepcion, Chile — We report a detailed study of the magnetic properties of Cu$_{1-x}$Co$_x$, with Co concentrations between 7 and 10 at% produced by mechanical alloying, through a reactive milling process by using a Retsch PM 400 planetary ball mill under argon atmosphere. We have magnetically characterized our samples by using a Vibrating Sample magnetometer, VSM, from Quantum Design. We conducted magnetization hysteresis loops at different temperatures from 5 to 300 K. We also measured magnetization as a function of temperature for samples with different milling times. We analyzed the dependence of the coercive field on temperature and found that when milling time increases from 80 to 100h, it reflects an increase in the coercive field from 425 to 525 Oe at 30K; that is the maximum coercive field observed on its multiferroic charateristics. Crystallographic structural, thermal, dielectric and magnetic properties are measured and discussed in terms of the dilution of magnetic Mn$^{3+}$ ions. Replacement of Mn$^{3+}$ ions with Ga$^{3+}$ changes the compound into a disordered multiferroic system and colossal magnetoelectric effect observed in DyMn$_2$O$_5$ disappears quickly below x<0.1 in DyMn$_{1-x}$Ga$_x$O$_5$. However as the content of Ga increases above x>0.1, a new type of ferroelectric transition identified by a peak in dielectric constant is evolved from the slowly varying dielectric background. Moreover remarkable enhancement of dielectric constant at ferroelectric transition temperature is continued even up to the solubility limit of Ga (x=0.2). This observation suggests a possible example of the channel for ferroelectricity in the disordered multiferroic system. K1.00089 Magnetic behavior of Mn$_{1-x}$Zn$_x$ Ferrite nanoparticles at low temperature. O. MARIN, D. REYES, Thin Films Group, Physics Department, Universidad del Valle, O. ALMANZA, Physics Department, Universidad Nacional de Colombia, P. PRIETO, Thin Films Group, Physics Department, Universidad del Valle, A. MENDOZA, Physics Department, Universidad Nacional de Colombia — We report on magnetic spin resonance and magnetization hysteresis loops of Mn$_{1-x}$Zn$_x$ Ferrite nanoparticles with sizes ranging from 20nm to 50nm obtained via microemulsions. The samples were evaluated by VSM technique ranging from 10K<300K at ZFC and FC. EPR measurements at T=180K were carried out in the 0 ≤ x ≤ 0.75 range. Experimental results for the peak-to-peak linewidth, $\Delta H_{pp}$, have been discussed by the existence of monodomain ferrimagnetic particles. The results indicate an increase of $\Delta H_{pp}$ by increasing the Zn concentration. The EPR signal shows a second EPR peak for x>0.5 at g=4.10 associated to local magnetic fields produced for Mn chains. The anisotropy constant was calculated by means of a genetic algorithm for parameter optimization of the Jiles-Atherton model.

This work was partially supported by COLCIENCIAS, under research Project No. 1106-05-11-458 Projects, and the Excellence Center for Novel Materials - CENM under COLCIENCIAS contract 043-2005.

K1.00090 ABSTRACT WITHDRAWN —
K1.00091 NMR and spin relaxation in systems with iron oxide nanoparticles . NATALIA NOGINOVA, TRACEE WEAVER, NSU, Norfolk, VA, ALEXANDR ANDREYEV, MARK FELCICIANO, OLHS, Virginia Beach, VA — Effect of the superparamagnetic nanoparticles to $^1$H NMR spectra and spin dynamics of the host systems have been studied in liquid (water and toluene), solid (polymer) and gelatin suspensions of $\gamma$-Fe$_2$O$_3$ nanoparticles. Significant broadening of $^1$H NMR spectra and growing relaxation rates were observed with increased concentration of nanoparticles in the liquid systems while the polymer systems demonstrate inhomogeneous broadening of the spectra and practically no dependence of $T_1$ upon the nanoparticle concentration. In gelatin solution, both effects were observed depending on the line position. We explain the experimental results taking into account predomination of self-diffusion as a source of the relaxation, with allowance made for the formation of magnetic aggregates.


1Research is supported by Fresno State CSM fund.

K1.00093 ABSTRACT HAS BEEN MOVED TO SESSION V32 —

K1.00094 Exchange biased anisotropic magnetoresistance in Co/CoO bilayer1, S. SAHOO, University of Nebraska-Lincoln, S. POLISETTY, YI WANG, T. MUKHERJEE, XI HE, CH. BINEK — We measured the anisotropic magnetoresistance of a Co(11nm)/CoO bilayer in exchange biased and unbiased states. The bilayer was fabricated on a-Al$_2$O$_3$ substrate maintained at 300°C by molecular beam epitaxy at a base pressure of 10$^{-11}$ mbar. θ-2θ X-ray diffraction scans reveal hcp (001) texture of the Co film. No peak associated with the naturally formed CoO top layer was identified. Small angle X-ray reflectivity scans yield the Co and CoO thicknesses as 11 and 2.4nm, respectively. Exchange bias was observed from field cooled magnetization measurements at various temperatures carried out in a closed cycle cryostat. Exchange bias varies quasi linearly with temperature and vanishes at the blocking temperature, $T_B$$=97K$. The latter is less than 2/3 of the bulk Neel temperature allowing to estimate the $T_0$ antiferromagnetic correlation length of Co to be 1.84 nm in accordance with the geometrical confinement.

1This work was supported by NSF through Career DMR-0547887, MRSEC DMR-0213808, and NRI.

K1.00095 Synthesis and characterization of iron nanoparticles by high-pressure sputtering. JEFFREY CARVELL, ELIJAH AIYETA, RIUHUA CHENG, Indiana University Purdue University Indianapolis — The study of magnetic nanoparticles is interesting because of its importance and applications in the production of nano-electromechanical systems (NEMS) and micro-electromechanical systems (MEMS). We use a sputtering technique to deposit iron nanoparticles on a silicon substrate. The nanoparticles are then analyzed using atomic force microscopy (AFM), x-ray diffraction, and superconducting quantum interference devices (SQUID). AFM data shows that the size of the particles depends on different deposition conditions. Then, x-ray diffraction data shows that the nanoparticles adopt the body-centered cubic crystal structure. Finally, SQUID measurements were performed to characterize the magnetic properties of the nanoparticles. Systematic change in the magnetic properties was observed for particles with different sizes. The results show that the size and magnetic properties could be tuned by changing the deposition conditions.

K1.00096 Magnetite-Alginate-AOT nanoparticles based drug delivery platform. R. REGMI, C. SU-DAKAR, A. DIXIT, R. NAIK, G. LAWES, Department of Physics and Astronomy, Wayne State University, U. TOTI, J. PANYAM, College of Pharmacy, University of Minnesota, R.P. VAISHNAVYA, Kettering University — Iron oxide having the magnetic structure is a widely used biomaterial, having applications ranging from cell separation and drug delivery to hyperthermia. In order to increase the efficacy of drug treatments, magnetite nanoparticles can be incorporated into a composite system with a surfactant-polymer nanoparticle, which can act as a platform for sustained and enhanced cellular delivery of water-soluble molecules. Here we report a composite formulation based on magnetite and Alginate-aerosol OT (AOT) nanoparticles formulated using an emulsion-cross-linking process loaded with Rhodamine 6G [1]. We prepared two set of nanoparticles by using Ca$^{2+}$ or Fe$^{3+}$ to cross-link the alginate polymer. Additionally, we added ∼8 nm diameter Fe$_3$O$_4$ magnetic nanoparticles prepared by a soft chemical method to these alginate-AOT nanoparticles. The resulting composites were superparamagnetic at room temperature, with a saturation magnetization of approximately 0.006 emu/g of solution. We will present detailed studies on the structural and magnetic properties of these samples. We will also discuss HPLC measurements on Rhodamine uploading in these composites. [1] M.D.Chavanpatil, Pharmaceutical Research, vol.24, (2007) 803.

K1.00097 The importance of local band effects for ferromagnetism in hole doped La$_2$CuO$_4$. BERNARDO BARBIELLINI, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA, THOMAS JARLBORG, DPMC, University of Geneva, CH-1211 Geneva 4, Switzerland — Doping is of vital importance for cuprates, since only about 0.15 holes per Cu atom is sufficient to transform them from antiferromagnetic insulators to the best known superconductors. The doping is usually made through substitution of the ternary element (Sr for La etc.), and the effects are typically described by rigid band filling of the CuO band. However, results of band calculations for supercells of La$_{2-x}$Ba$_x$CuO$_4$ show that the rigid band model for doping is less adequate than what is commonly assumed. In particular, weak ferromagnetism (FM) can appear locally around $T_B$ and vanishes at the blocking temperature, $T_B$, because of its importance and applications in the production of nano-electromechanical systems (NEMS) and micro-electromechanical systems (MEMS). We use a sputtering technique to deposit iron nanoparticles on a silicon substrate. The nanoparticles are then analyzed using atomic force microscopy (AFM), x-ray diffraction, and superconducting quantum interference devices (SQUID). AFM data shows that the size of the particles depends on different deposition conditions. Then, x-ray diffraction data shows that the nanoparticles adopt the body-centered cubic crystal structure. Finally, SQUID measurements were performed to characterize the magnetic properties of the nanoparticles. Systematic change in the magnetic properties was observed for particles with different sizes. The results show that the size and magnetic properties could be tuned by changing the deposition conditions.

K1.00098 Tuning magnetic interaction in orthorhombic Neodymium-Yttrium-Manganites Nd$_{1-x}$Y$_x$MnO$_3$. SVEN LANDGESSELL, DIMITRI ARGYRIOU, NADIR ALIOUANE, Hahn-Meitner-Institut — By lowering the Mn-O-Mn bond angle in LnMnO$_3$ with Ln=La-Ho the Neel-temperature decreases and at $T_N$=Th the A-type antiferromagnet transforms to an incommensurate (IC) spin-spiral phase for $T_N$=Gd, Tb, Dy. The spin-spiral breaks both inversion and time reversal symmetry leading to a strong coupling between magnetism and ferroelectric polarization. We investigate the evolution of the magnetic and structural from the A-type phase to the IC spin spiral phase by systematically replacing neodymium by yttrium in NdMnO$_3$ resulting to a decrease of the tolerance factors to values similar to that for multiferroic TbMnO$_3$. One advantage of this approach is that the tolerance factor can be tuned and that neodymium and yttrium are not high neutron absorbing elements in sharp contrast to other rare earths like Gd, Dy and Eu. Compositions $x$=0.0 have been prepared, neutron and x-ray powder diffraction patterns were measured as well as the magnetic properties. It can be shown that by decreasing the tolerance factor that way, similar effects can be seen as with varying the ionic size of the rare earth ions. For example we found that between 0.4 $<$ $x$ $<$ 0.6 the incommensurate phase co-exists with the A-type antiferromagnetic phase and with $x$=0.6 and higher the system is only incommensurate and seemingly multiferroic.
K1.00099 Determination of Magnetic Directions in Multiferroic BiFeO$_3$ Thin Films, M.B. HOLCOMB, L.W. MARTIN, Y.H. CHU, UC Berkeley, A. SCHOLL, E. AREN HOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, S.Y. YANG, T. CONRY, Q. HE, R. RAMESH, UC Berkeley — BiFeO$_3$ (BFO), a ferroelectric and an antiferromagnet, is the only single phase room temperature multiferroic that is currently known. Multiferroics are interesting materials not only because of their exciting order parameters, but also for the potential for parameter coupling. In order to understand the magnetoelectric coupling, the individual order parameters must first be understood. A combination of in-plane and out-of-plane piezoresistance force microscopy (PFM) allows 3D mapping of the ferroelectric polarization directions in micron-sized regions of the films. The magnetic order of BFO was obtained by using x-ray linear and circular dichroism imaging using a photoelectron emission microscope (PEEM). Angle dependent structural measurements allow decoupling of the two order parameters, ferroelectric and magnetic, contributing to the photoemission signal. Careful analysis of linear and circular dichroism images at critical angles allows determination of magnetic directions in BiFeO$_3$. These studies reveal a strain-driven reduction in magnetic symmetry in thin films, leading to the formation of an easy magnetic axis as opposed to the observed easy plane for bulk films. This reduction along with the previous proof of FE-AM coupling allows electrical control of its magnetic axis.

K1.00100 Magnetization damping in epitaxial CrO$_2$ (110), HWACHOL LEE, KRISHNA CHETRY, CLAUDIA K.A. MEWES, ARUNAVA GUPTA, TIM MEWES, Center for Materials for Information Technology — Epitaxial CrO$_2$ thin films were grown on TiO$_2$ (110) substrates using chemical vapor deposition (CVD) using a CrO$_2$ precursor as described elsewhere [1]. In-plane angular dependent ferromagnetic resonance (FMR) measurements confirm a uniaxial in-plane anisotropy with the easy axis along the c-axis. Frequency dependent FMR measurements were carried out over a frequency range from 7-60 GHz along the easy axis of the film. The resonance field dependence on the microwave frequency is well described by the Kittel formula, enabling the determination of M$_c$ and γ of the films. The ferromagnetic resonance linewidth depends only weekly on the microwave frequency: the linewidth has a minimum around 20 GHz and increasing linearly for larger frequencies with a very small slope. Based on this we estimate the Gilbert damping constant (intrinsic) to be of the order 10$^{-4}$, i.e. very small. The main contribution to the magnetization relaxation is extrinsic in nature and can therefore be further optimized. References: [1]: X. W. Li, A. Gupta, and G. Xiao, Appl. Phys. Lett. 75, 713 (1999).

K1.00101 Magnetic Clustering and Possible Chemical Nonuniformity in Bi0.125Ca0.875MnO3, YUHAI QIN, TREVOR TYSON, New Jersey Institute of Technology — The manganite system Bi$_{3-x}$Ca$_x$MnO$_3$ possesses intriguing properties in the low bismuth doping region. In this electron doped region ($0.6<c<1$), a large ferromagnetic (FM) moment of $\sim 1.2$ Bohr magnetons per Mn site is found for $c<0.875$. However, the origin of this FM clustering configuration is still an open question. Chemical nonuniformity (Bi ion segregation) as a candidate interpretation has been explored with TEM/EDS, which can give a quantitative assessment of geometrical parameters, chemical composition and crystal structure of second phase particles. We have identified evidences for the possible Bi nonuniformity in nano-scale, which are consistent with the results from small-angle neutron scattering. This work is supported by NSF DMR-0512196.

K1.00102 ABSTRACT WITHDRAWN —

K1.00103 Zero and low field magnetization dynamics in tapered nanopillar spin valves caused by micromagnetic structure, P.M. BRAGANCA, O. OZATAY, O.J. LEE, D.C. RALPH, R.A. BUHRMAN, Cornell University — Exciting spin-torque driven magnetization dynamics in a uniformly magnetized nanomagnet typically requires large magnetic fields and electric currents, both of which are undesirable for practical applications. Here, we show that by combining an angled sidewall and a low saturation magnetization material, such as permalloy (Py), in a simple nanopillar spin valve structure, a micromagnetic configuration can be established which is conducive to spin-torque excitation of magnetization dynamics in the absence of an external magnetic field. As verified by micromagnetic simulations, these magnetization oscillations occur in both nanomagnet layers of the spin valve due to a substantial out of plane magnetization component that is located at and near the ends of the tapered elliptical disks. For magnetic fields close to zero, the resultant giant magnetoresistance spectra show oscillations with peak frequencies between 5.2-6.5 GHz, and minimum linewidths on the order of 50 MHz.

K1.00104 Non-Adiabatic Spin Transfer Torque in Realistic Materials, ION GARATE, ALLAN MACDONALD, University of Texas at Austin — The motion of simple domain walls and more complex magnetic textures in the presence of a transport current is sensitive to the size and sign of the non-adiabatic spin transfer torque coefficient $\beta$, even though this dimensionless coefficient is believed to typically have a small value. The ratio of $\beta$ to the Gilbert damping coefficient $\alpha$ is particularly important and has been variously estimated to be close to 0, close to 1, and large or small. By identifying $\beta$ as following from the influence of a transport current on $\alpha$, we derive concise analytical expressions for $\beta$ in real materials. When spin-orbit is included in the band structure, the damping has an intra-band contribution that is proportional to the square of the quasiparticle lifetime. We will discuss estimates for $\beta$ and for the $\alpha/\beta$ ratio in common magnetic materials.

K1.00105 Study of Fe/Cr Magnetic Multilayers and Periodic Arrays of Submicron Magnetic Dots by Vector Network Analyzer Technique, FARKHAD ALIEV, JUAN FRANCISCO SIERRA, AHMAD AWAD, VLADIMIR PRYADUN, Universidad Autonoma de Madrid, Spain, GLEB KAKAZEI, INSTITUTE OF MAGNETISM NASU, Kiev, Ukraine — Vector network analyzer (VNA) technique up to 8.5 GHz was applied to measure in-plane dynamic response in Fe/Cr magnetic multilayers and for the in-plane magnetized periodic arrays of Permalloy circular magnetic dots. In the antiferromagnetically coupled [Fe/Cr]$_n$, multilayers ($n=10,20,40$) we have investigated field dependence of the acoustic resonance in a wide range of temperatures between 300K down to 2K both for the low magnetic fields and close to the saturation field. FMR studies of the array of FeNi dots with diameter of 1 micron, the aspect ratio L/R=0.1 and with centre to centre distance varying between 1.2 to 2.5 micron allowed to resolve multiple FMR resonances as a function of magnetic field. We have found the main FMR linewidth to be dependent on the magnetic history. For the magnetic fields below 300 Oe, where magnetic vortex state forms, we have observed the field dependence of the radial modes ($f_r > 6$GHz) to show minima close to the zero magnetic field.

K1.00106 Ferromagnetic Resonance in Magnetic and Conducting Thin Films1, TOM GEORGE, University of Nebraska, Lincoln, JUSTIN BAIZE, MIRCEA CHIPARA, The University of Texas Pan American, RALPH SKOMSKI, DAVID J. SELLMYER, University of Nebraska, Lincoln — Ferromagnetic resonance provides unique information concerning both electronic spin orientation and their interactions. A model for the simulation of magnetic resonance line shape in metallic and magnetic thin films, developed within the thermodynamic approximation is presented. The proposed model includes the contribution of the Gilbert term to the precession of magnetic moments in external magnetic fields, the effect of shape anisotropy, of magnetocrystalline anisotropy, and allows for different textures. The main features of the ferromagnetic resonance line (line position, line width, line asymmetry, and line shape) are analyzed while taking into account the competition between magnetic and conducting features. The model allows a detailed analysis of the angular dependence of the ferromagnetic resonance line. It has been tested on a multilayer consisting of 60 bilayers (Fe 0.16 nm/Pt 0.18 nm).

1ESR measurements were done within the laboratory of Professor A. Rajca from the Chemistry Department of the University of Nebraska Lincoln.
K1.00107 Optical control of topological spin and charge transport in semiconductors, WANG YAO, ALLAN MACDONALD, QIAN NIU, The University of Texas at Austin — In n-doped semiconductors, the strong spin-orbit coupling in valance band can be utilized through the band renormalization by optical field off-resonantly coupled to the interband transitions. The adiabatic electronic ground state is thus reactively controlled by optical pulses, exhibiting an anomalous spin-dependent Hall conductivity. Light-matter interaction is exploited here in a unique way, i.e., light does not induce real excitations in the system but act as a control knob for switching on/off novel material properties, in contrast to most previous use of light. With the control by linearly polarized light, a pure spin Hall current of electrons can be driven by an in-plane DC electric field, which results in net spin accumulations at the edges of the optical excitation area. Effectively, one has created a spin battery powered by optical pulses together with DC electric field, or equivalently, an optically gated spin transistor. As conduction band spin-orbit coupling is not needed, the resultant electron spin accumulations can have long lifetime when control light is adiabatically switched off. In addition, circularly polarized light breaks the time reversal symmetry and can result in spin polarized anomalous Hall conductance.

K1.00108 Ultrafast Photoinduced Ferromagnetic Phase Enhancement in Ion Implanted GaMnAs, INGRID COTOROS, University of California at Berkeley, Berkeley CA 94720, JIGANG WANG, Lawrence Berkeley National Laboratory, Berkeley CA 94720, PETER STONE, OSCAR DUBON, DANIEL CHEMLA, University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley CA 94720, MIKE D. COHEN, Department of Physics, MIT, 98 E. St., Cambridge, MA 02139, USA — First-principles relativistic band calculations for platinum, which is one of the most important materials for metallic SHE and spintronics. We find that intrinsic spin Hall conductivity (SHE) is as large as \( \sim 2000 \, h/e \, (\Omega \cdot cm)^{-1} \) at room temperature, and decreases down to \( \sim 200 \, h/e \, (\Omega \cdot cm)^{-1} \) at low temperature. It is due to the resonant contribution from the spin-orbit splitting of the doubly degenerated \( d \)-bands at high-symmetry \( L \) and \( X \) points near the Fermi level. By modeling these near-degeneracies by an effective Hamiltonian, we show that SHE has a peak near the Fermi energy and that the vertex correction due to impurity scattering vanishes. We therefore argue that the large SHE observed experimentally in platinum is of intrinsic nature. \[1\] G.Y. Guo, S. Murakami, T.-W. Chen, and N. Nagaosa, arXiv:cond-mat/07050409.

K1.00109 Intrinsic spin Hall effect in platinum metal, GUANG-YU GUO, Department of Physics, National Taiwan University, Taipei 106, Taiwan, SHUCHII MURAKAMI, Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan, TSUNG-WEI CHEN, Department of Physics, National Taiwan University, Taipei 106, Taiwan, NAO TO NAGAO, Department of Applied Physics, University of Tokyo, 113-8656, Japan — Spin Hall effect (SHE) is studied with first-principles relativistic band calculations for platinum, which is one of the most important materials for metallic SHE and spintronics. We find that intrinsic spin Hall conductivity (SHE) is as large as \( \sim 2000 \, h/e \, (\Omega \cdot cm)^{-1} \) at room temperature, and decreases down to \( \sim 200 \, h/e \, (\Omega \cdot cm)^{-1} \) at low temperature. It is due to the resonant contribution from the spin-orbit splitting of the doubly degenerated \( d \)-bands at high-symmetry \( L \) and \( X \) points near the Fermi level. By modeling these near-degeneracies by an effective Hamiltonian, we show that SHE has a peak near the Fermi energy and that the vertex correction due to impurity scattering vanishes. We therefore argue that the large SHE observed experimentally in platinum is of intrinsic nature. \[1\] G.Y. Guo, S. Murakami, T.-W. Chen, and N. Nagaosa, arXiv:cond-mat/07050409.

K1.00110 First-principles Study on the Magnetic Interaction in ZnO-based Dilute Magnetic Semiconductors, MASAYUKI TOYODA, The Institute of Scientific and Industrial Research, Osaka University, HISAZUMI AKA, Graduate School of Science, Osaka University, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA, The Institute of Scientific and Industrial Research, Osaka University — Using first-principles calculations, we investigate the electronic structures and magnetic properties of dilute magnetic semiconductors (DMS). The electronic structures are calculated by using Korringa-Kohn-Rostoker method combined with the coherent potential approximation. Since the d electrons of the magnetic impurity in DMS are strongly localized, we apply self-interaction correction to the local density approximation for the exchange-correlation energy. From the first-principles results, we evaluate the magnetic exchange interaction \( J_{ij} \) between the pairs of magnetic impurities by using the Lichtenstein’s formula. We found that the magnetic interaction in ZnO-based DMS is basically antiferromagnetic without any additional carrier because of large energy gaps between the occupied and unoccupied d states. We will also discuss about the carrier dependence of the magnetic interaction in ZnO-based DMS.

K1.00111 Corresponds between Spin-Hall Effect and Ordinary Hall Effect, ROKSANA GOLIZADEH-MOJARAD, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN-47906, USA — The “spin-Hall effect” has recently attracted a lot of attention and a central question is whether the effect is due to the intrinsic spin-orbit interaction or due to spin-asymmetric scattering by extrinsic impurities. We shed light on this question using a new approach based on the non-equilibrium Green function (NEGF) formalism, which allows us to go continuously from the ballistic to the diffusive limit and we present approximate analytical expressions that describe our results fairly well. We establish a correspondence between Spin Hall effect and Ordinary Hall effect, since from our point of view these two effects are quite similar. Our model suggests that a spin accumulation proportional to the current should be observed in clean ballistic samples and we show how this spin accumulation evolves as momentum and/or spin relaxation processes are introduced in a controlled way. We further show good quantitative agreement with recent experimental observations in GaAs suggesting that this can be understood in terms of an intrinsic effect driven by the Rashba interaction, although experiments on ZnSe likely have a different origin.

K1.00112 Anisotropy, coercivity and thermal activation in \( L_{10} \)-FePt Nanoparticles, CHUANBING RONG, NARAYAN POUYDAL, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019 — \( L_{10} \) FePt materials have attracted tremendous attention for their potential applications due to their high anisotropy and excellent mechanical properties. It is well known that the magnetization behavior of small particles is strongly affected by thermal fluctuation especially when the particle size is close to the critical size of superparamagnetic. In this work, the size effect on anisotropy constant \( K_u \), magnetic viscosity parameter \( S \), activation volume \( V_{ac} \), and coercivity \( H_c \) of the \( L_{10} \) FePt nanoparticles obtained by ion-beam sputtering have been investigated. The maximum field-dependent coercivity parameter \( S_{max} \) increases monotonously with temperature for the particles with size of 3 nm to 8 nm. Moreover, \( S_{max} \) of small particles is more sensitive to temperature than that of large particles. However, the temperature dependence of both \( S_{max} \) and \( V_{ac} \) of the 15 nm particles are different from those for 3-8 nm particles. Further analysis of relation between \( H_c \) and \( V_{ac} \) suggested that the 3-8 nm particles are ideal single-domain particles, while the 15 nm particles can not be well described as single-domain particles even the particle size is much smaller than the single-domain size.

K1.00113 Composition Dependent Properties in Disordered, Lower Dimensional Co/Ni Dichloride Monohydrate, G.C. DEFOITIS, E.S. VOS, A.H. HOPKINSON, W.M. MAY, T.M. OWENS, C.M. DAVIS, C.L. DESANTO, College of William and Mary — This new mixed magnet is composed of the lower dimensional insulators Co dichloride monohydrate and Ni dichloride monohydrate, both studied previously by us. The Co system is an antiferromagnetic singl band with an antiferromagnetic transition at 15.0 K and a spin glass transition at 8.4 K. The antiferromagnetic Ni system orders at 5.6 K. Both materials are characterized by ferromagnetic intrachain interactions and antiferromagnetic interchain interactions; an element of randomness is present in the Co system but not the Ni. Mixtures of these two components have been prepared and studied over a wide composition range. The variation in magnetic behavior with composition is not anticipated on the basis of pure component properties, e.g., the location of a susceptibility maximum and of a field induced transition. Irreversibility effects are present over a broad composition range. It seems likely that admixture of the two components enhances effects of disorder and frustration already present in the Co system, so that equilibrium behavior occurs even for Ni rich mixtures.

Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research.
K1.00114 Generic and topological features of flat bands in tight binding hopping models, DORON BERGMAN, Yale University, CONGIUN WU, University of California, San Diego, LEON BALENTS, University of California, Santa Barbara — We study some generic features of flat bands, that appear in a number of tight binding hopping models. Such models have recently received some attention in the literature [1,2], with a number of suggested experimental realizations. In some models the flat band touches dispersing bands at a discrete set of high-symmetry points in the Brillouin zone. In other models, the flat band is gapped. A topological argument, crucially depending on the boundary conditions of the system, which explains why in some models the flat band is gapped, while in others it is not. The argument is based on the observation that in flat bands in addition to quasi-local eigenstates, there invariably exist states involving non-contractible loops. In those cases where the flat band touches a dispersive band, our argument also determines at which points in momentum space this occurs. [1] C. Wu, et al., Phys. Rev. Lett. 99, 070401 (2007) [2] J. Schulenburg, et al., Phys. Rev. Lett. 88, 167207 (2002)

K1.00115 Magnetic Behavior in Cobalt and Nickel Dibromide Hydrates1, G.C. DEFOTIS, C.M. DAVIS, C.L. DESANTO, College of William and Mary — The magnetism of 3d transition metal dibromide hydrates has been examined far less than for corresponding chlorides. Continued here is a program of examining the especially neglected monohydrate systems, by extending earlier studies of Co and Ni dichloride monohydrates to bromide counterparts. For comparison purposes the only lightly examined Co and Ni dibromide hydrate systems are also studied. Both Ni materials, dihydrate and monohydrate, show an antiferromagnetic susceptibility maximum at, surprisingly, virtually the same 6.0 K location. The maximum is broader and of lesser magnitude in the monohydrate, perhaps indicating lower dimensional character. Marked differences in magnetization isotherms as a function of temperature also distinguish these two materials. In Co dibromide dihydrate a susceptibility maximum occurs at 9.5 K, only about half the temperature of a similar feature in the corresponding chloroide. Yet in the monohydrate an enhanced susceptibility maximum appears at 15.9 K, remarkably close to such a feature in the corresponding chloride. And as in that system, nonequilibrium magnetic properties appear, suggesting that a significant degree of frustration is present.

1Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research.

K1.00116 Raman spectroscopy of multiferroic TbMnO3J, J. R. SIMPSON, A. R. HIGHT WALKER, NIST, Gaithersburg, MD 20899, R. VALDÉS AGUILAR, A. B. SUSHKOV, H. D. DREW, University of Maryland, College Park, MD 20742, S. PANKRATS, Y. J. CHOI, C. ZHANG, S.-W. CHEONG, Rutgers University, New Brunswick, NJ 08854 — Coupling between the lattice and magnetic degrees of freedom in TbMnO3 has been observed to produce magnetic excitations with electric dipole activity, or electromagnons. Recent reports of electromagnons in other multiferroic (113)-orthomanganites and related (125)-manganites indicate a complementary Raman study may provide additional insight into the importance of spin-lattice coupling. We present Raman spectra of single-crystal and polycrystalline TbMnO3 using a triple-grating spectrometer in a collinear backscattering configuration as a function of temperature (4 − 300 K) and polarization along various crystallographic axes. The absence of any observable low-frequency modes (intensity $\sim 1000$ times that of prominent Raman-active phonons) suggests a weak scattering cross-section for the electromagnon. Additionally, we discuss the temperature dependence of Raman-active phonons and compare with results from infrared measurements.

1Work supported, in part, by the NIST-NRC postdoctoral fellowship.


K1.00117 Magnetic behaviour of the Bi$_{1-x}$Sr$_x$Ir$_2$O$_7$ pyrochlore, CARLOS COSIO-CANESTEDO, OLIVER MARTINEZ-ANAYA, GUSTAVO TAVIZON, Facultad de Quimica, PABLO DE LA MORA, Facultad de Ciencias, FRANCISCO MORALES-LEAL, ROBERTO ESCUDERO, Instituto de Investigaciones en Materiales — Compounds of the Bi$_{1-x}$Sr$_x$Ir$_2$O$_7$ solid solution have been synthesized by the solid state reaction method. Structural modifications as well the valence states of Iridium have been studied as a function of the strontium content by Rietveld refinements and electrochemical analytical methods. Electrical properties of Bi$_{1-x}$Sr$_x$Ir$_2$O$_7$ show single phase and metallic behaviour in the whole range of compositions. Magnetically this system behaves as a Curie-Weiss paramagnet from 2-300 K. The magnetic moment suggests the presence of Ir$^{3+}$ valence state.

K1.00118 Invar effect and non-collinear magnetism in CuFe alloys, MARCUS EISENBACH, G. MALCOLM STOCKS, Oak Ridge National Laboratory, Oak Ridge, TN — The Invar effect has been observed in many Fe rich alloys, most famously Ni Invar. Generally the Invar behavior is associated with the strong coupling between the lattice and magnetic degrees of freedom, and therefore depends on the magnetic ordering in these alloys. Recent experimental works observed an Invar effect in fcc-CuFe solid solutions. [Gorria et al., PRB 69, 214421 (2004)] We investigate the magnetic states of fcc-CuFe solid solutions in the Invar regime and compare it with the order in low Fe concentration alloys, to establish the connection between the Invar effect and the magnetic order. To study this we employ the locally selfconsistent multiple scattering (LSMS) real space method for solving the LDA Kohn-Sham equation as well as its extension to fully relativistic calculations to investigate all effects leading to anisotropies and non collinear ordering of magnetic moments.

K1.00119 X-ray scattering study of the magnetic phase transitions in GdFe3(BO3)4, H. MO, C.S. NELSON, Brookhaven National Laboratory, Upton, NY 11973, L.N. BEZMATERIALYK, V.L. TEMEROV, Kirenskioe Institute of Physics, Russian Academy of Science, Akademgorodok, Krasnoyarsk, 660036 Russia — The rare earth iron borates have interesting magnetic properties due to the subtle interactions between the rare earth and the iron moments. Among these materials, GdFe3(BO3)4 has the most complex phase diagram as suggested by previous studies. [1,2] These studies suggest that iron moments order antiferromagnetically below $T_N \approx 36$ K and that there are several additional magnetic phase transitions below $T_N$. Yet whether and at what temperature the Gd moments order and the nature of the additional transitions, remain largely unknown. Using x-ray magnetic scattering, we have verified that the moments order antiferromagnetically with a propagation vector $(0 \ 0 \ 3/2)$. Large resonant scattering enhancements at the Gd $L_{11}$ and $L_{21}$ edges show unambiguously that Gd moments order at $T_N$. Both resonant and nonresonant scattering data exhibit a splitting of the magnetic peak along $c^*$ above $\sim 10$ K which indicates an incommensurate phase transition, with the incommensurability $\delta$ increasing continuously as a function of temperature ($\delta \sim 0.038$ near $T_N$). Use of the NSLS/BNL is supported by the U. S. DOE under Contract no. DE-AC02-98CH10886. [1] F.-Y. Chen et. al, PRB 73, 54435 (2006)


K1.00119 X-ray scattering study of the magnetic phase transitions in GdFe3(BO3)4, H. MO, C.S. NELSON, Brookhaven National Laboratory, Upton, NY 11973, L.N. BEZMATERNYKH, V.L. TEMEROV, Kirenskioe Institute of Physics, Russian Academy of Science, Akademgorodok, Krasnoyarsk, 660036 Russia — The rare earth iron borates have interesting magnetic properties due to the subtle interactions between the rare earth and the iron moments. Among these materials, GdFe3(BO3)4 has the most complex phase diagram as suggested by previous studies. [1,2] These studies suggest that iron moments order antiferromagnetically below $T_N \approx 36$ K and that there are several additional magnetic phase transitions below $T_N$. Yet whether and at what temperature the Gd moments order and the nature of the additional transitions, remain largely unknown. Using x-ray magnetic scattering, we have verified that the moments order antiferromagnetically with a propagation vector $(0 \ 0 \ 3/2)$. Large resonant scattering enhancements at the Gd $L_{11}$ and $L_{21}$ edges show unambiguously that Gd moments order at $T_N$. Both resonant and nonresonant scattering data exhibit a splitting of the magnetic peak along $c^*$ above $\sim 10$ K which indicates an incommensurate phase transition, with the incommensurability $\delta$ increasing continuously as a function of temperature ($\delta \sim 0.038$ near $T_N$). Use of the NSLS/BNL is supported by the U. S. DOE under Contract no. DE-AC02-98CH10886. [1] F.-Y. Chen et. al, PRB 73, 54435 (2006)

K1.00120 Non-Collinear Magnetic Orderings in Mott Insulators, ALEXANDER BAZHAN1, P.L. Kapitza Institute for Physical Problems, RAS. — Non-collinear magnetic orderings of four Cu magnetic moments in Mott insulators R$_2$Cu$_2$O$_4$ (R = Nd, Pr) of I4/mmm symmetry and associated magnetic phase transitions are of interest in studies of transformations, when correlated electron-hole carriers are introduced in R$_2$-xCe$_x$Cu$_2$O$_4$. Orderings are determined by thermodynamic potential in representation by antiferromagnetic I$_1$, I$_2$, and magnetic m vectors, with orderings of I$_1$, I$_2$, vectors along [100], [010] axis, with values $I_1^2 = I_2^2 = 1/2$, $m^2 = 1$ [1], which can be presented as, $I_1 = 1/2$ A($I_1^2 + I_2^2$) + 1/2 A($I_1^2 - I_2^2$) + 1/4 $I_1^2$ + $I_2^2$ + 1/4 $I_1^2$ + 1/4 E ($I_1^2 - I_2^2$) + 1/4 a ($I_1^2 + I_2^2$) + 1/4 b ($I_1^2 + I_2^2$) + 1/4 c ($I_1^2 + I_2^2$) · m with $I_1 = 0$. Magnetic phase transitions, are concerned with change of I$_1$, I$_2$ values in fields ~H$_{-1}$, ~H$_{+1}$, where $I_1^2 = 0$, $I_2^2 = I_2^2$, when field is oriented along [100], [110] axis respectively, and next I$_2$ orientation to orthogonal to field direction in fields ~H$_{-1}$, ~H$_{+1}$, when field is along [110] axis. Fields H$_{-1}$, H$_{+1}$ are presented as, H$_{-1}$ = 2BE$_2$; H$_{+1}$ = H$_{+1}$, if H$_{+1}$ = b$_{+1}$BE$_1$, H$_0^2$ = -2H$_{+1}$H$_{-1}$ if H$_{+1}$ = b$_{+1}$BE$_1$. Formation of charge density waves of checkerboard structure can be detected by studies of transformation of magnetic phase transitions and fields in R$_2$-xCe$_x$Cu$_2$O$_4$. [1] A. N. Bazhan, AIP Proceedings 850 (2006) 1241

1 K1.00121 CHEMICAL PHYSICS —

K1.00122 CHEMICAL PHYSICS

K1.00122 An Explanation for the Very Low Friction of Polyelectrolyte Brushes, JEFFREY SOKOLOFF, Northeastern University — It is shown using a method based on the mean field theory of Miklavcic Marcella that it should be possible for osmotic pressure due to the counterions associated with the two polyelectrolyte polymer brush coated surfaces to support a reasonable load (i.e., about 10$^{15}$ Pa) with the brushes held sufficiently far apart to prevent entanglement of polymers belonging to the two brushes, thus avoiding what is believed to be the dominant mechanisms for static and dry friction. This is shown to be true even if the brushes are highly compressed, which is consistent with the observation by Raviv, et. al., that the friction for polyelectrolyte brush coated surfaces can be exceedingly low, even if the brushes are highly compressed.

K1.00124 Temperature Dependent Raman Intensities and Calculations of Chiral ketone Conformers, WATHEQ AL-BASHEER, The Hashemite University, Zarqa 13115, JUN LI, Pacific Northwest National Laboratory, Richland, WA 99352, ROBERT COMPTON, The University of Tennessee, Knoxville, TN 37996 — Vibrational Raman spectra for the C-H stretch region of 3-methylcyclopanetane (R3MCP) neat sample as a function of temperature variation will be presented and employed as a conformational analysis method. Probing the methyl group C-H stretch region (2850 – 3000 cm$^{-1}$) relative peak intensities of assigned conformers, is being manipulated to determine the conformer energy differences between equatorial methyl and axial methyl isomers. Raman spectroscopy performed under liquid nitrogen temperatures (LN) will also be presented as a preliminary tool to observe Raman vibrational modes at liquid nitrogen temperatures (~ 77 K), and to improve resolution and high signal to noise ratio. An observed few wavenumbers bathochromic (red) shift in Raman lines frequencies will be attributed to sample phase change. The validity of Density Functional Theory (DFT) calculations, of different levels basis sets, for R3MCP conformers Raman intensities and frequencies will be investigated and compared against experimental findings.

K1.00125 Optimum Atomic Ranges in Coupled Dipole Method, HYE-YOUNG KIM, ZACHARY BOND, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA — In recent years, the coupled dipole method (CDM) has been applied to calculate the van der Waals dispersion interaction (VDW) between dielectric nanoclusters. Similar self-consistent method has also been used to calculate the static polarizabilities, from which the fully-retarded VDW was calculated. The breakthrough in CDM is that it can calculate all n-body terms in VDW. This allows for significant improvement upon the usual 2-body description of VDW. As the size of nanoclusters close to the experimentally measurable size, however, solving for eigenvalues of a large matrix (with all n-body interactions) in CDM becomes non-trivial. Since each interaction term decreases as the separation distance becomes large, certain atomic ranges within which the VDW would converge is expected in large systems. Identifying this range will improve the efficiency of CDM. Here, we report the results of a systematic study on the optimized maximum atomic ranges in CDM for different shapes and sizes of clusters. REF: Langmuir 23, 1735 (2007).

1 Work supported by the U. S. Department of Energy Basic Energy Sciences grant DOE-FG02-07ER46414 and conducted at the Center of Nanophase Materials Sciences, which is sponsored at Oak Ridge National Lab by the Division of Scientific User Facilities, DOE.

K1.00126 Umbrella Sampling in the Long Range Ising Model, RANJIT CHACKO, HARVEY GOULD, Clark University, WILLIAM KLEIN — Umbrella sampling with the largest cluster size as the local order parameter has been used to study liquid to solid nucleation. In the absence of a rigorous definition of a solid-like cluster, an ad hoc definition of the clusters must be adopted. As a result it is not clear if the vanishing of the free energy barrier found by umbrella sampling should be interpreted in terms of a spinodal and how well the cluster found at the free energy maximum corresponds to the true nucleating droplet. To better understand umbrella sampling with a local order parameter we study nucleation in the long-range Ising model for which the cluster definition is given rigorously by a percolation mapping. We determine the free energy of the long-range Ising model as a function of the largest cluster size and the quench depth, and study the properties of the nucleating clusters as the spinodal is approached.

K1.00127 TOF MS Study of Photodissociation of Borazine at 193 nm, DACHUN HUANG, VLADIMIR MAKAROV, Univ of Puerto Rico, Dept of Chem, ARTURO HIDALGO, Univ of Puerto Rico, Dept of Phys, BRAD WEINER, Univ of Puerto Rico, Dept of Chem, GERARDO MORELL, Univ of Puerto Rico, Dept of Phys — Photofragmentation of borazine molecule has been investigated in a supersonic molecular beam condition (Ar + 1% borazine mixture) by using radiation of 193 nm (250 mJ/pulse). Fragments were photo ionized using another laser (193 nm, 3 mJ/pulse) and detected by a linear time-of-flight mass spectrometer. Both lasers passed through the work area of the TOF mass spectrometer at the same time. We found that the main channel of borazine photofragmentation is formation of B$_3$H$_4$ radical and hydrogen atom. The possible mechanism was proposed and discussed.
K1.00128 Single Pulse Time Resolved Four Wave Mixing. YEHIAM PRIOR, YURI PASKOVER, ILYA SH. AVERBUKH, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — We present a new experimental technique for single-shot time resolved ultrafast Coherent Anti-Stokes Raman Spectroscopy (CARS), where we use the arrival time of pulses at the intersection of broad beams as controlled time delays. The three dimensional (Bovacs) phase-matching configuration allows unique mapping of two independent time delays (pump-Stokes and pump-probe) onto the geometrical axes of the interaction region. The signal emitted from each point of the beams’ intersection carries information on the molecular state at the particular time delay after the excitation, and thus the spatial profile of the CARS beam provides time resolved trace of the intra-molecular vibrational dynamics. We show that our technique allows for capturing of a few picoseconds of vibrational evolution by means of a single ultrashort pulse. Moreover, the ability to resolve two time delays between pulses enables us to study vibrational dynamics on the ground and the excited electronic states, as well as the correlation between the nuclear motions within these different vibrational potentials. The ability to record vibrational dynamics while the molecules freeze to the single molecule to a optical pulse allows for characterization of short living and unstable chemical species as transitional complexes of chemical reactions.

K1.00129 Spectroscopic characterization of the ionization energy, \( \Sigma^+_g \), \( (2)\Pi^+ \), and \( (3)\Pi \) states of Be \(_g\). JEREMY MERRITT, Department of Chemistry, Emory University, Atlanta GA 30322, VLADIMIR BONDBYBEY, Institut fur Physikalische und Theoretische Chemie der TU Munich, Garching, Germany, MICHAEL HEAVEN, Department of Chemistry, Emory University, Atlanta GA 30322 — Low-lying electronic states of beryllium dimer are investigated by laser induced fluorescence (LIF) and resonance enhanced multiphoton ionization (REMPI) spectroscopies. \( \text{Be}_2 \) is formed by pulsed laser ablation and free jet expansion into vacuum. Comparing 1+1 REMPI and LIF spectra for the \( \Sigma^+_g \) (v=0) \( \rightarrow \) \( \Pi^+_g \) (v) bands we find significant perturbations in the REMPI spectra, which are interpreted as autoionizing resonances in the ionization continuum. Photoionization efficiency (PIE) measurements yield an accurate value for the ionization energy, namely 7.40 eV, which is considerably larger than previous theoretical predictions. New CASSCF/MRCI calculations are presented which accurately reproduce the experimental IP. Rotationally resolved spectra for the \( (1)\Sigma^+_g \rightarrow (2)\Pi_1 \) and \( (1)\Sigma^+_g \rightarrow (3)\Pi \) band systems of \( \text{Be}_2 \) have also been measured for the first time providing further experimental benchmarks for recent ab initio calculations. PIE measurements are also used to accurately determine the \( \Sigma^+_g < \rightarrow (1)\Pi_1 \) interval.

K1.00130 Rovibrationally Inelastic Velocity-Dependent Cross Sections from Doppler Lineshapes. PAULA MATEI, STEVEN COPPAGE, BRIAN STEWART, Wesleyan University — We are studying rovibrationally inelastic processes in the Li\(_g\) (A) – noble gas system through a spectroscopic technique that employs the Doppler shift for velocity selection of the lithium molecules. Our goals are to look for experimental evidence of a novel vibrational transfer mechanism that involves impacts with the side of the molecule, and to investigate and compare different combinations of rotational and vibrational energy transfer. The experimental results will be compared with cross sections calculated from ab initio potential surfaces.

K1.00131 Saturated nucleate pool boiling of oxygen under magnetically-enhanced effective gravity\(^1\). T. A. CORCOVILOS\(^2\), M. E. TURK\(^3\), California Institute of Technology - Division of Physics, Math. and Astronomy, Pasadena, CA, USA, D. M. STRAYER, California Institute of Technology - Jet Propulsion Laboratory, Pasadena, CA, USA, N. N. ASPLUND, N.-C. YEH, California Institute of Technology - Division of Physics, Math. and Astronomy, Pasadena, CA, USA — We investigate the effect of enhancing gravity on saturated nucleate pool boiling of oxygen for effective gravities \( (g^e) \) of 1g, 6g, and 16g \( (g = 9.8 \text{ m s}^{-2}) \) at a saturation pressure of 760 torr and for heat fluxes of 10 \( \sim \) 3000 W m\(^{-2}\). The effective gravity on the oxygen is increased by applying a magnetic body force generated by a superconducting solenoid. We measure the heater temperature (expressed as a reduced superheat) as a function of heat flux and fit this data to a piecewise power-law/linear boiling curve. At low heat flux \( (\sim 100 \text{ W m}^{-2}) \) the superheat is proportional to the cube root of the heat flux. At higher heat fluxes, the superheat is a linear function of the heat flux. The value of the transition heat flux separating these two regions is proportional to \( \sqrt[3]{g^e} \), indicating a possible link to the critical heat flux.

\(^1\)Funding by NASA
\(^2\)Current address: Rice University, Houston, TX, USA
\(^3\)Current address: Cornell University, Ithaca, NY, USA

K1.00132 Thermal Hysteresis in Magnetic Phases of Solid Oxygen. N. S. SULLIVAN, University of Florida, M. PILLA, Triquint Semiconductor Inc., J. A. HAMIDA, University of Florida — Measurements of the dielectric susceptibility of solid oxygen have been carried out in the temperature range 4.2 \( \sim \) 54 K. Relatively large hysteresis effects \( (~0.4\%) \) have been observed for the dielectric response in the \( \alpha \) and \( \beta \) phases on thermal cycling below 44 K. The temperature for the transition between the two-sublattice antiferromagnetic \( \alpha \) phase and the frustrated quasi-helical \( \beta \) phase is observed to be independent of the thermal cycles. The areas of the thermal hysteresis scale with the extent of the thermal excursion in the frustrated \( \alpha \) phase.

K1.00133 Does Hot Water Freeze Faster than Cold? Investigation of the Reproducibility and Causes of the Mpemba Effect. JOSEPH THOMAS, SUSAN LEHMAN, The College of Wooster — An investigation into the reproducibility and possible causes of the Mpemba effect has been performed. The Mpemba effect is the name given to the common observation by non-scientists that hot water appears to freeze faster than cold water.\(^1\) Previous scientific studies of this effect have found conflicting results. These discrepancies appear to be due in part to inconsistent definitions of freezing based on visual observation. We have investigated the Mpemba effect by continuously monitoring the temperature of a container of water to determine the amount of time needed for the water to turn completely to ice, as indicated by the temperature falling below 0 °C. We have successfully observed the effect repeatedly and have found it to be dependent on the sample’s temperature history rather than the sample temperature when placed into the freezer. Room temperature water which had been briefly heated to 100 °C then cooled froze approximately 50 % faster than room temperature water which had not been heated. The effect on the freezing time of increasing or decreasing the amount of dissolved gas in the water will also be discussed. 1. M. Jeng. Am. J. Phys. 74 514 (2006).

K1.00134 Surface roughness effects on superhydrophobicity. CHUNYANG YANG, UGO TARTAGLINO, BO PERSSON, IFF, FZ-Juelich, D-52425, Germany — Superhydrophobic surfaces, with liquid contact angle greater than 150 degree, have important practical applications ranging from self-cleaning window glasses, paints, and fabrics to low friction surfaces. Many biological surfaces, such as the lotus leaf, have hierarchically structured surface roughness which is optimized for superhydrophobicity through natural selection. Here we present a molecular dynamics study of liquid droplets in contact with self-affine fractal surfaces. Our results indicate that the contact angle for nanodroplets depends strongly on the root-mean-square (rms) surface roughness amplitude but is nearly independent of the fractal dimension of the surface\(^2\). References: [1] C. Yang, U. Tartaglino and B.N.J. Persson, Phys. Rev. Lett. 97, 116103 (2006) [2] C. Yang, U. Tartaglino and B.N.J. Persson, arXiv:0710.3264
K1.00135 Production of Polymer Core-Shell Colloids with High Uniformity via Coaxial Electrospay. YOUN KYUN HWANG, UNYONG JEONG, Department of Materials Science and Engineering, Yonsei University, Seoul — Although nanofibers fabricated by electrospinning have been attracting wide interest, the production of colloids by electrospaying has not much studied so far. We have developed a simple method for the production of core-shell colloids with high uniformity by means of the coaxial electrospay. Contrary to usual coaxial setup, the inner nozzle was set to touch the inside wall of the outer nozzle for reproducible production. A polymer solution for the core was introduced through the outer nozzle and another solution for the shell was provided through the inner nozzle. The structure of the colloids was dependent on the polymer concentration, relative feed ratio between the polymer solutions. Especially, core-shell structured colloids are our primary interest due to their promising uses in drug-delivery systems, cosmetics, and food industries. This talk will present the production of core-shell colloids consisting of two polymer components.

K1.00136 Janus particles at the planar water-oil interface. QIAN CHEN, SHAN JIANG, STEVE GRANICK, University of Illinois at Urbana-Champaign — Amphiphilic Janus particles (hydrophobic on one side, hydrophilic on the other) were placed at the planar water-oil interface at various surface coverage and found to self-assemble into two-dimensional crystals with long-range hexagonal order, which we studied by fluorescence and phase contrast microscopy. Surprising dependence is observed not only on the surface chemical makeup of the hydrophilic side but also on the Janus balance (i.e. the relative sizes of hydrophobic and hydrophilic portions), which is analogous to the HLB balance that characterizes molecular surfactants.

K1.00137 Ab Initio Simulations of Silica Alpha Quartz Surfaces and their Interaction with Water1, YUN-WEN CHEN, HAI-PING CHENG, Quantum Theory Project, Department of Physics, University of Florida — Two types of dry silica alpha quartz (0001) surfaces have been investigated through density functional calculations. One is the dense surface proposed by Rignanese et al. [1] that has 3-fold flower like six-member rings on the top and the three-member rings underneath. The other one is a newfound surface that has zigzag-shape six-member rings on the top and the three-member rings underneath. It is found that the new one is energetically more stable than the dense surface. The interactions of the surfaces with water molecules have also been concerned. Both of the surfaces have the similar hydrophilic properties. We report our results from MD simulations at a temperature of 300K.


1 Funded by NSF Grant 0403871

K1.00138 Molecular motion in alkylsilane self-assembled monolayers1, DERRICK STEVENS, North Carolina State University (NCSU), MARY SCOTT, LAURA GUY, JASON BOCHINSKI, LAURA CLARKE, NCSU — We have investigated intra-molecular rotation within polar-substituted alkylsilane self-assembled monolayers (SAMs) on fused silica, utilizing surface-sensitive dielectric spectrosopy. Both trichlorosilanes (which allow crosslinking within the SAM) and monochlorosilanes (attached only to the surface) are utilized to grow monolayer and submonolayer films. Dielectric loss spectra as a function of temperature have been obtained for SAMs with varying carbon chain length, surface coverage, and alkyl terminal group. As shown by ellipsometry, contact angle measurements, and AFM, monochlorosilanes form a more disordered monolayer than trichlorosilanes. This more disordered film may result in additional degrees of freedom within the monolayer, or in the language of phase transitions, a rotator phase. Issues such as uncontrolled vertical polymerization and film growth by island formation and their effect on rotational dynamics will be discussed.

1 Funded by NSF Grant 0403871

K1.00139 Photoemission and reaction study of mass-selected Pt clusters on TiO2(110) surface, NORITAKE ISOMURA, YOSHIHIDE WATANABE, Toyota Motor Corporation, Toyota Central R&D Labs., Inc. — Metal cluster ions were produced by a DC magnetron-sputter cluster ion source [1] with an ion funnel [2], the surface. Catalytic properties of mass-selected metal clusters on well-defined oxide surfaces have been investigated using the new ultra high vacuum cluster ion source. One is the dense surface proposed by Rignanese et al. [1] that has 3-fold flower like six-member rings on the top and the three-member rings underneath. The other one is a newfound surface that has zigzag-shape six-member rings on the top and the three-member rings underneath. It is found that the new one is energetically more stable than the dense surface. The interactions of the surfaces with water molecules have also been concerned. Both of the surfaces have the similar hydrophilic properties. We report our results from MD simulations at a temperature of 300K.


K1.00140 Structural and electronic properties of aluminum nanoclusters1, MRUDULA RAPARLA, TUNNA BARUAH, University of Texas at El Paso, RAJENDRA ZOPE, University of Texas at El Paso — The electronic properties of Al clusters containing up to 60 atoms are investigated using an all electron density functional theory using large polarized Gaussian basis sets with 39 Gaussians per atom (NRLMOL basis). We have performed an extensive search for the lowest energy isomers for clusters up to Al21. We build a database of candidate structures for the ground state using different strategies. First, a few structures are randomly generated and fully relaxed using planewave pseudopotential method. We also performed simulated annealing runs using ab initio molecular dynamics for clusters up to Al20. In three sets of simulated annealing runs the clusters were heated up to 900 and 1000K and were slowly cooled to 50K at different rates. After every half picosecond, the cluster was quenched. Additionally the best basin hopping geometries obtained using empirical embedded atom potential were also fully optimized. The process generates 40-50 structures for each size. All the structures are relaxed using empirical embedded atom potential. The calculated electron affinities and theoretical photoelectron binding energies are in very good agreement with experiment. Theoretical predictions for Zn, Ca and Cs anions display additional electron detachment binding energies that are not present in the published experimental data.

[1] Acknowledgment: Grant Teragrid PHY050026

K1.00141 Density Functional Study of the Photodetachment Spectra of Zinc and Calcium Cluster Anions1, YAFEI DAI, E. BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — The structure and electronic states of zinc cluster anions Zn3 through Zn6 and calcium cluster anions from Ca2 through Ca19 were optimized within the hybrid density functional approach. Based on these results, the photodetachment spectra of Zn3 through Zn6 and of Ca3 through Ca4 anions were determined. Additionally, the electron affinity of Zn, (N up to 9) and of Ca (N up to 19) was calculated within the same approximation. Both the calculated electron affinities and theoretical photoelectron binding energies are in very good agreement with experiment. Theoretical predictions for Zn, Ca2 and Ca4 anions display additional electron detachment binding energies that are not present in the published experimental data.

[1] Acknowledgment: Grant Teragrid PHY050026

K1.00142 Amorphous and crystallographic structures of TiO2(110) surfaces and their interaction with water, JUN-CHAI KIM, SANGHO JUNG, Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology, Ulsan — The TiO2(110) surface is a model system for understanding the basic properties of amorphous titanium dioxide, the most important component of a number of chemical and physical systems such as catalysts, non-destructive diagnostics, and thin film solar cells. This talk will present the construction of a database of candidate structures for the ground state at various surface coverage using an all electron density functional theory. The database is then used to study the interaction between the water molecules and the TiO2(110) surface. The interaction energy profiles are calculated for various water molecules and the adsorption geometry is determined for each water molecule. The results are compared with the experimental data to evaluate the extent to which the theoretical predictions are in agreement with experiment.

K1.00143 Production of Polymer Core-Shell Colloids with High Uniformity via Coaxial Electrospay. YOUN KYUN HWANG, UNYONG JEONG, Department of Materials Science and Engineering, Yonsei University, Seoul — Although nanofibers fabricated by electrospinning have been attracting wide interest, the production of colloids by electrospaying has not much studied so far. We have developed a simple method for the production of core-shell colloids with high uniformity by means of the coaxial electrospay. Contrary to usual coaxial setup, the inner nozzle was set to touch the inside wall of the outer nozzle for reproducible production. A polymer solution for the core was introduced through the outer nozzle and another solution for the shell was provided through the inner nozzle. The structure of the colloids was dependent on the polymer concentration, relative feed ratio between the polymer solutions. Especially, core-shell structured colloids are our primary interest due to their promising uses in drug-delivery systems, cosmetics, and food industries. This talk will present the production of core-shell colloids consisting of two polymer components.

K1.00136 Janus particles at the planar water-oil interface. QIAN CHEN, SHAN JIANG, STEVE GRANICK, University of Illinois at Urbana-Champaign — Amphiphilic Janus particles (hydrophobic on one side, hydrophilic on the other) were placed at the planar water-oil interface at various surface coverage and found to self-assemble into two-dimensional crystals with long-range hexagonal order, which we studied by fluorescence and phase contrast microscopy. Surprising dependence is observed not only on the surface chemical makeup of the hydrophilic side but also on the Janus balance (i.e. the relative sizes of hydrophobic and hydrophilic portions), which is analogous to the HLB balance that characterizes molecular surfactants.

K1.00137 Ab Initio Simulations of Silica Alpha Quartz Surfaces and their Interaction with Water1, YUN-WEN CHEN, HAI-PING CHENG, Quantum Theory Project, Department of Physics, University of Florida — Two types of dry silica alpha quartz (0001) surfaces have been investigated through density functional calculations. One is the dense surface proposed by Rignanese et al. [1] that has 3-fold flower like six-member rings on the top and the three-member rings underneath. The other one is a newfound surface that has zigzag-shape six-member rings on the top and the three-member rings underneath. It is found that the new one is energetically more stable than the dense surface. The interactions of the surfaces with water molecules have also been concerned. Both of the surfaces have the similar hydrophilic properties. We report our results from MD simulations at a temperature of 300K.


1 Funded by NSF Grant 0403871
K1.00142 Ligand-spacer controlled size selectivity of gold clusters1, GHAZAL SHAFAI, SAMPYOO HONG, TALAT RAHMAN, University of Central Florida, MASSIMO BERTINO, Virginia Commonwealth University — It has been observed in the experiment that the presence of diphosphine ligands with varying spacers (L1, L5, and L8) leads to the formation of Au clusters of characteristic size [1]. In particular, in the presence of L1, Au11 clusters are formed, while the presence of L5 leads to the formation of Au42, Au42, and Au14 clusters. We have carried out calculations based on the density functional theory in the projector augmented wave scheme (PAW) and the pseudopotential approach, to examine the effect of the diphosphine ligand spacer size on the stability of Au clusters containing 2 to 11 atoms through evaluations of the cluster total energy and proper corrections of spurious interactions between charged supercells. For example, to investigate the stability of Au11, we compare the total energy of Au11(X)2 and Au8(X)2 + Au4X4⁻ (X=L1, L3, or L5 ligands) and find that Au11 is indeed preferred by L1 rather than L5, in agreement with the experiment. The structural electronic changes brought about by the various local environments of these clusters are presented with full details. [1] Bertino et al. Phys. Chem. B Lett. 110, 21416 (2006)

1Work supported in part by DOE grant DE-FG02-03ER46354.

K1.00143 An excitonic state-resolved approach to coherent phonons in quantum dots: generation and relaxation dynamics. RYAN COONEY, D.M. SAGAR, SAMUEL SEWALL, PATANJALI KAMBHAMPATI, McGill University — The strength of exciton-phonon couplings in quantum dots has remained controversial due in part to the complex eigenstate spectrum of electrons and holes in these systems. We recently implemented a combined time/frequency domain approach, towards exciton selective spectroscopy. This approach initially yielded a unified picture of the controversial mechanism of electron and hole relaxation dynamics in quantum dots. Recently, this approach yielded the first simultaneous observation of underdamped coherent optical and acoustic modes, thereby providing a direct measure of the controversy size dependent exciton-phonon coupling strengths for both modes. Pumping into higher excited states reveals that the Auger based electron relaxation process is vibrationally incoherent whereas non-adiabatic dynamics retain a memory of the vibrational coherence. Finally, phase and state-selective results reveal the electronic surface upon which the vibrational coherence is generated.

K1.00144 ABSTRACT WITHDRAWN

K1.00145 Photochemical Processing of Carbon Dioxide Ices and Simple Ice Mixtures1, T. RANDY DILLINGHAM, DAVID CORNELISON, Northern Arizona University — The investigation of the photochemical processes that can occur in carbon dioxide ices and ice mixtures have important applications in astrophysics, planetary astronomy, and atmospheric chemistry. In this investigation, carbon dioxide ices and ice mixtures are grown at various temperatures using a closed-cycle helium cryostat. The ices are irradiated with x-rays for periods of up to six hours. The chemical changes that occur during the processing are monitored using x-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy. A quadrupole mass spectrometer is also used to study the gas phase species evoking from the ice surface during photoprocessing. The XPS, FTIR and mass spectrometer results are presented and correlated. It is noted that significant differences are observed, particularly for the time dependence of the evolution of the gas phase molecules, between ices grown at 77 K as compared to those grown at 20 K and at intermediate temperatures.

1Supported by the NASA Space Grant Program

K1.00146 Single Electron Transport of Oligothiophene molecules1, TOSHIFUMI TERUI, National Institute of Information and Communications Technology, YUTA KO NOGUCHI, Center of Frontier Science, Chiba University, TAKUYA KATAYAMA, MICHI O MATSUSHITA, Grad. Sch. of Arts and Sci, University of Tokyo, RIEKO UEDA, National Institute of Information and Communications Technology, TADASHI SUGAWARA, Grad. Sch. of Arts and Sci, University of Tokyo — We examined the fabrication of single-electron transistors (SETs) with oligothiophene derivative or Au nanoparticle covered with oligothiophene as Coulomb island. The SET device was consists of a nanogap electrode, a molecular Coulomb island, and back gate electrode. The nanogap electrode was fabricated by the electromigration method. We could obtain the SET characteristics from the electron transport properties of both devices at 11 K. Spectra that owing to a molecule was obtained in the electric transport properties of these devices. Moreover, we could obtain the SET characteristics in some devices.

1This work was supported by the Grant-in-Aid for Scientific Research on the Priority Area “Application of Molecular Spins from Nanomagnets to Biological Spin Systems” by the Ministry of Education, Culture, Sports, Science and Technology of Japan.

K1.00147 Characterization of hydroxyls on Si(001)-2×1:H2O using O 1s core-level spectroscopies and core-excited state DFT calculations, STEPHANE CARNIATO, Universite Pierre et Marie Curie, SYLVIE RANGAN, University of Texas at Dallas, JEAN-JACQUES GALLET, FRANCOIS ROCHET, GEORGES DUFOUR, FABRICE BOURNEL, Universite Pierre et Marie Curie, ALBERTO VERDINI, LUCA FLOREANO, TASC-INFN National Laboratory — The Si(001)-2×1 surface exposed to water molecules at room temperature has been chosen to single out the electron structure of the hydroxyl Si-OH, a surface species playing an important role in many technologically relevant processes. We confront here original core-electron spectroscopy DFT calculations to O 1s XPS (X-ray Photoelectron Spectroscopy) and NEXAFS (Near Edge Absorption Fine Structure) data. On various Si-OH environments (unpaired and paired hydroxyls), the impact of hydrogen bond on the calculated core-ionized and/or neutral core-excited states is examined, and compared to the limit case of the water dimer. The theoretical approach enables to label the main experimental NEXAFS transitions and to interpret their polarization-dependent dichroism. As water dissociation on the surface can go beyond the formation of hydroxyls, the vibrational coherence is generated.

K1.00148 Structure-Property Relations in beta-Hairpin Peptide Hydrogels, ROHAN HULE, DARRIN POCHAN, Materials Science and Engineering, University of Delaware — A de novo designed beta hairpin peptide, capable of undergoing intramolecular folding and consequent intermolecular self-assembly into a fibril-based network that forms a hydrogel, has been studied. A combination of SANS and cryo-TEM have been used to quantitatively investigate the nanofibrillar hydrogel network morphology. An increase in the peptide concentration resulted in a denser fibrillar network as revealed via a change in the high q mass fractal exponent from 2.5 to 3. This is accompanied by a decrease in the measured correlation length from 23 to 16 Angstroms, indicative of the increase in the number of crosslinks and a reduction in the interfibril distances in the proximity of individual crosslinking points. In the USANS regime, a slope of -4 is indicative of gel microporosity. These changes, both, at the network as well as the individual fibril length scales can be directly visualized in situ by cryo-TEM. Fibrillar nanostructure and the network morphology are directly related and can be used to tune the bulk hydrogel stiffness, as studied via oscillatory rheology. Knowledge of the precise nano-through microstructure can help in the formation of specific structure-property relationships in these novel peptide-based hydrogels.
K1.00149 Structured Hydrogels using Micelles as Templates, WONJOO LEE, PETER KOFINAS, ROBERT M. BRIBER, University of Maryland, College Park — Moleculearily imprinted polymers can be created by crosslinking polymers in the presence of molecular templates. If the pores generated after the removing of templates have almost the same size and shape as the template, the material has a potential to be used for separation, biosensor and drug delivery applications. In this work, micelles were used as the template as they can be easily removed from the hydrogel and a range of structures are accessible by combining a (linear) polyelectrolyte and an oppositely charged surfactant. Poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA) was synthesized and quaternized using methyl iodide. We have performed small angle neutron scattering (SANS) on solutions and hydrogels of PDMAEMA with sodium dodecyl sulfate (SDS) under different concentrations and crosslinking densities, and then performed the dynamic light scattering (DLS) and transmission electron microscopy (TEM). The results were confirmed by the SANS and DLS measurements. The PDMAEMA solution which contained SDS was dispersed as rod-like micelle-like structures coated with the SDS molecules. The micelle-like structures were associated along the polymer chain in a head-to-head structure consistent with what has been observed in the (uncharged) poly(ethylene oxide)/SDS system. Furthermore, we also show the interaction between PDMAEMA and micelles is strong enough to maintain the nanoscale structure formed along the PDMAEMA chain, even after crosslinking, leading to a structured hydrogel.

K1.00150 Controlled Charge-Flow in A Molecular Interferometer, SPIROS SKOURITSIS, Department of Physics, University of Cyprus, Nicosia 1678, Cyprus, DEQUAN XIAO, Department of Chemistry, Duke University, Durham, NC 27708, DAVID BERATAN, Department of Chemistry and Biochemistry, Duke University, Durham, NC 27708 — We describe an electron transfer molecule interferometer capable of controlling electron flow by inelastic tunneling manipulation. The molecule consists of electron donor and acceptor groups that are connected by a bridge. Upon photo-excitation of the molecule, an electron transfers from the donor to the acceptor group by tunneling through the bridge. The structure of the bridge is such that it provides interfering electron tunneling pathways. We show how to control interferences between the pathways by isotopic substitutions of pathway-specific bridge atoms. Such substitutions create pathway-localized bridge vibrations that can be selectively IR-excited during the electron transfer event. We suggest ways of experimentally controlling pathway interferences and electron transfer rates.

K1.00151 Single-crystalline rutile TiO$_2$ nanowires by mass selected Ni catalyst: Synthesis and electrical properties, MYUNG HWA KIM, CHRISTOPHER LARSON, JEONG MIN BACK, XIHONG CHEN, MARTIN MOSKOVITS, ALEC WODTKE, Department of Chemistry & Biochemistry, University of California at Santa Barbara — We present a novel method for growing high quality TiO$_2$ nanowires using mass-selected Ni clusters of nanometer sizes produced by magnetron sputtering and also show their electric field-effect functions. Single-crystalline TiO$_2$ nanowires (NWs) are grown by atmospheric pressure physical vapor deposition (APVVD) process, using TiO and Ti metal powders as a Ti source and Ni nanoparticles as a catalyst, respectively. For the TiO NWs growth, first, the Ti metal layer with a thickness of $\sim$50 nm was then deposited on the SiO$_2$/Si substrate by the e-beam evaporation technique and subsequently, the mass selected Ni clusters by using magnetron sputtering source combined with a quadrupole mass filter was deposited onto the Ti layer. APPVD growth was then performed in a horizontal quartz tube furnace at 800 °C–850°C by introducing high purity Ar carrier gas (99.999%) with the flow rate of 300 sccm for 2 hours. The $I-V$ curves are linear over the entire annealing temperature range at 200 °C–500°C, showing that the electrodes form good ohmic contacts with the nanowires. The $I$ vs $V$ curves for various values of $V_{SD}$ and gate dependent $I-V$ curves of a TiO$_2$ nanowire configured as a back-gated FET are also obtained and will be discussed.

K1.00152 Accurate electronic-structure description of Mn complexes: A GGA+U approach, ELISE Y. Li, Chemistry, Massachusetts Institute of Technology, HEATHER KULIK, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Conventional density-functional approach often fail in offering an accurate description of the spin-resolved energetics in transition metals complexes. We will focus here on manganese (Mn) complexes, where Mn has the possibility to change its electronic configuration. Using an accurate method, we determine the electronic structure of these evolving complex (OEC) of photosystem II and the manganese catalysis (MC). We apply a self-consistent GGA + U approach [1], originally designed within the DFT framework for the treatment of strongly correlated materials, to describe the geometry, the electronic and the magnetic properties of various manganese oxide complexes, finding very good agreement with higher-order ab-initio calculations. By considering the different oxidation states of dinuclear systems containing the [Mn$_2$O$_2$]$^{2+}$ (n = 2, 3, 4) core, are investigated, in order to mimic the basic face unit of the OEC complex [1]. H. J. Kulik, M. Cococcioni, D. A. Scherlis, N. Marzari, Phys. Rev. Lett., 2006, 97, 103001

K1.00153 A density functional theory study of the benzene-water complex, SHEN LI, VALENTINO COOPER, Department of Physics and Astronomy, Rutgers, The State University of New Jersey, T. THONHAUSER, Department of Physics and Astronomy, Rutgers The State University of New Jersey and Department of Materials Science and Engineering, MIT, AARON PUDDER, Department of Physics and Astronomy, Rutgers, The State University of New Jersey and Lawrence Livermore National Laboratory, DAVID LANGRETH, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — We calculated the intermolecular interaction of the benzene-water complex using real-space pseudopotential density functional theory with a van der Waals density functional (vdW-DF). Developed recently, vdw-DF has been applied to a number of van der Waals complexes with promising results. Our results for the intermolecular potential energy surface between benzene and a water molecule clearly show a stable configuration with the water molecule standing above the benzene with one or both of the H atoms pointing toward the benzene plane, as predicted by previous studies. However, when the water molecule is pulled outside the perimeter of the benzene ring, the configuration of the complex becomes unstable with the water molecule attaching in a saddle point configuration to the rim of the benzene with its O atom adjacent to a benzene H. The results for ground state structure are compared with available experiments and quantum chemical calculations.

K1.00154 First-principles study of the oxygen-reduction reaction on the Pt (100) surface, EUNJIA KIM, TAO PANG, Department of Physics and Astronomy, University of Nevada, Las Vegas — We have performed density-functional study of oxygen-reduction reaction on the Pt(100) surface. Equilibrium structures of oxygen on the surface are found and carefully analyzed. Our calculations show that oxygen molecules reside in the small terrace of the complete (100) surface. The adsorption of oxygen on Pt(100) is exothermic by $\sim$0.2 eV per oxygen atom. More oxygen molecules reaching the surface will continue to reduce but also drive the ones in the monolayer away from the surface, making the surface an effective catalyst. However, oxygen does not stack up into layers on the Pt(100) surface and therefore does not play a significant role in degrading the Pt (100) surface during any catalytic process there.

K1.00155 Chromium of Model Organic Aerosol$^1$, ANGELA RINCON, CALTECH, MARCELO GUZMAN, HARVARD UNIVERSITY, MICHAEL HOFFMANN, AGUSTIN COULISSI, CALTECH — The optical properties of the atmospheric aerosol play a fundamental role in the Earth’s radiative balance. Since more than half of the aerosol mass consists of complex organic matter that absorbs in the ultraviolet and visible regions of the spectrum, it is important to study the optical properties of the organic compounds. Here we report studies on the chromism vs. chemical composition of photolyzed (lamba longer than 305 nm) solutions of pyruvic acid, a widespread aerosol component, under a variety of experimental conditions that include substrate concentration, temperature and the presence of relevant spectator solutes, such ammonium sulfate. We use high resolution mass- and 13C NMR-spectrometries to track the oxidation state of the aerosol. First, we find that the aerosol undergoes a significant change in the UV-Vis spectrum when the aerosol is photolyzed with biologically active light of 212 nm. Subsequently, we study the effect of the aerosol’s chromism on its photobleaching properties. Since the chemical identity of the components of these mixtures does not change in these cycles, in which photobleached solutions gradually recover their yellow color in the dark with non-conventional kinetics typical of aggregation processes, we infer that visible absorptions likely involve the intermolecular coupling of carbonyl chromophores in supramolecular assemblies made possible by the polyfunctional nature of the products of pyruvic acid photolysis.

$^1$Supported by NSF grant ATM-0714329
K1.00157 Spatially separating individual conformers of neutral (bio)molecules. JOCHEN KÜPPER, FRANK FILSINGER, UNDINE ERLÉKAM, GERT VON HELDEN, GERARD MEIJER, Fritz-Haber-Institut der MPG, Berlin, Germany — Large (bio)molecules exhibit multiple conformers (structural isomers), even under the cold conditions present in a supersonic jet. For various applications, i.e., scattering experiments, it would be highly desirable to prepare molecular packets of individual conformers. It is well-known that polar molecules can be manipulated using strong electric fields. Many techniques have been developed for the manipulation of small molecules in low-field-seeking quantum states. However, application of these techniques to large molecules is not straightforward, because, for larger molecules, all states are high-field seeking at the relevant electric field strengths. To manipulate the motion of large molecules one has to use Alternate Gradient (dynamic) focusing. This method has been successfully demonstrated in the Alternate Gradient deceleration of diatomic molecules. Using the same Alternate Gradient focusing principle, applying switched electric fields in a quadrupole guide, we have set up a new experiment to spatially separate individual conformers of large molecules. This experiment exploits the different mass-to-dipole $(m/q)$ ratios, similar to a quadrupole mass-to-charge $(m/q)$ filter for ions. In a proof-of-principle experiment, we have demonstrated the conformer selection of cis- and trans-3-aminophenol.

K1.00158 Spectroscopy of free radicals and radical containing entrance-channel complexes in superfluid helium nanodroplets. JEREMY MERRITT, Department of Chemistry, University of North Carolina - Chapel Hill, JOCHEN KÜPPER, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany, ROGER MILLER, Department of Chemistry, University of North Carolina - Chapel Hill — The unique properties of superfluid helium nanodroplets, namely their low temperature (0.4 K) and fast cooling rates ($10^{15}$ K$^{-1}$), provide novel opportunities for the formation and high-resolution study of metastable structures or molecular complexes containing free radicals. We discuss methods for the production of radicals and their applicability for embedding the radicals in helium nanodroplets. The spectroscopy of free radicals (i.e., $\text{C}_2\text{H}_4$) and of radical containing entrance-channel complexes, for example $\text{X}–\text{HY}$ ($\text{X}=\text{Cl, Br, I, CH}_3$, $\text{Y}=\text{F, CN}$), embedded in helium nanodroplets is detailed. The observed complexes provide new information on the potential energy surfaces of several fundamental chemical reactions and on the intermolecular interactions present in open-shell systems. Prospects for further experiments of radicals embedded in helium droplets are discussed.

K1.00159 Calculation of spin-orbit, static polarizabilities, and alignment of cold polar molecules. OLIVIER DULIEU, MIREILLE AYMAR, Laboratoire Aime Cotton, CNRS, Univ Paris-Sud Orsay, France, JOHANNES DEIGLMAYR, ROLAND WESTER, MATTHIAS WEIDEMÜLLER, Albert-Ludwigs-University Freiburg, Germany — Cold polar molecules offer exciting perspectives for studying strongly open-shell systems. Prospects for further experiments of radicals embedded in helium droplets are discussed.

K1.00160 Comparison of molecular energies calculation using simulated quantum algorithm and classical computer methods. JOSEPH LESNIAK, Department of Electrical and Computer Engineering, Wichita State University, ELIZABETH BEHRMAN, Department of Physics, Wichita State University, MELVIN ZANDLER, Department of Chemistry, Wichita State University, PREETHIKA KUMAR, Department of Electrical and Computer Engineering, Wichita State University — Very few quantum algorithms are currently usable today. When calculating molecular energies, using a quantum algorithm takes advantage of the quantum nature of the algorithm and calculation. A few small molecules have been used to show that this method is possible. This method will be applied to larger molecules and compared to classical computer methods.

K1.00161 SEMICONDUCTORS

K1.00162 Growth and characterizations of m-plane GaN and InN on gamma-LiAlO$_2$ substrate grown by plasma-assisted molecular beam epitaxy. LI-WEI TU, Z. L. LEE, Y. T. LIN, C. Y. HO, Y. L. CHENG, K. L. WU, Z. H. GONG, B. H. TSENG, M. C. CHOU, National Sun Yat-Sen University, Taiwan, Q. Y. CHEN$^1$, University of Houston, H. W. SEO, University of Arkansas, W. K. CHU, University of Houston — Non-polar nitrides are investigated in this report. Substrate used is gamma-phase LiAlO$_2$ (LAO) (100) grown by Czochralski pulling method. The in-plane lattice mismatch between the LAO (100) plane and the GaN (1-100) plane, is small with a lattice mismatch of $0.3\%$ and $[1120]$GaN$\parallel[001]$LAO $\sim 1.7\%$. M-plane GaN epilayer and InN were successfully grown by ultra-high vacuum plasma-assisted molecular beam epitaxy system. Extensive characterizations have been carried out which include x-ray diffraction theta-two-theta scan, rocking curve measurement, scanning electron microscopy, cathodoluminescence, photoluminescence, and Raman spectroscopy. Details will be presented.

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K1.00163 AlGAN/GaN high electron mobility transistor grown on GaN template substrate by molecule beam epitaxy system$^1$. JENN-KAI TSAI, Center for General Education, National Formosa University, Hu-Wei, Yun-Lin, Taiwan 63208, R.O.C., Y. L. CHEN, M. H. GAU, W. Y. PANG, Y. C. HSU, IKAI LO, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China, C. H. HSIEH, Institute of Material Science and Engineering, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China — In this study, AlGAN/GaN high electron mobility transistor (HEMT) structure was grown on GaN template substrate by molecule beam epitaxy (MBE) equipped with an EPI UNI-Bulb nitrogen plasma source. The undoped GaN template substrate was grown on c-sapphire substrate assisted metal organic vapor phase epitaxy (MOVPE) using a 50 mTorr nitrogen plasma source. After growth of MOVPE and MBE, the samples are characterized by double crystal X-ray diffraction (XRD), transmission electron microscopy (TEM), field emission scanning electron microscopy (SEM), atomic force microscopy (AFM), and Hall effect measurements. We found that the RMS roughness of template substrate play the major role in got the high value of mobility on AlGAN/GaN HEMT. When the roughness was lower than 0.77 nm in a 25 $\mu$m x 25 $\mu$m area, the mobility of HEMT at the temperature of 77 K was over $10^{000}$ cm$^2$/Vs.

$^1$The authors would like to acknowledge Epistar corporation for supply GaN template substrates and financial support from the National Science Council of Republic of China.
The role of oxygen vacancies and defects on Lithium intercalation capacity of composite vanadium-titanium oxide thin films. M.B. SAHANA, C. SUDAKAR, C. THAPA, G. LAWES, K.R. PADMANABHAN, R. NAID, Dept. of Physics and Astronomy, Wayne State University, Detroit, MI 48201 USA, G. AUINER, Dept Electrical and Computer Engineering, Wayne State University, Detroit, MI 48202 USA, V.M. NAID, Dept of Natural Sciences, University of Michigan-Dearborn, Michigan 48128 — Composite films of vanadium-titanium oxide have been recognized as promising cathode materials for lithium ion batteries. While there is a consensus agreement that the cycling stability of the mixed V/Ti-oxide system is improved compared to V_2O_5 thin films, there are different findings on the Li+_ intercalation capacity of V_2O_5, PCCM Institute, Princeton University.

Fe-Doped SnO Powders Obtained By Sol-Gel Method, Mechanochemical Alloying, and Thermal Treatment. JAIME OSORIO, ANA CALLE, JAILES BELTRAN, LUIS SANCHEZ, Universidad de Antioquia, LILIANA TIRADO, Universidad del Quindio, KIYOSHI NOMURA, University of Tokyo, CESAR BARRERO, Universidad de Antioquia, ESTADO SOLIDO TEAM, OPTOELETRONICA TEAM, APPLIED CHEMISTRY SCHOOL OF ENGINEERING TEAM — The present work is aimed to investigate experimental conditions to obtain pure SnO_2 and FeSnO_2 powder by three methods: (1) sol-gel method, (2) mechanochemical alloying and (3) thermal treatment. In (1), different precursors were employed: mixtures of Sn^{4+} and Fe^{3+} or Sn^{2+} and Fe^{2+}. In (2), SnO_2 and α-Fe or α-FeO_2 were used as reactants. In (3), the Fe-doped SnO_2 were obtained by mechanochemical milling and thermal treatment. All samples were characterized by X-ray diffraction (XRD) using Rietveld refinement, Fourier-transformed infrared (FTIR) spectroscopy and room temperature 57Fe Mössbauer spectrometry (MS). The XRD patterns of samples prepared by (1) showed only peaks of SnO_2. The MS showed ferromagnetic and paramagnetic signals. The samples obtained by (2) showed XRD peaks due to SnO_2 (rutile). The MS revealed the presence of Fe^{2+} and Fe^{3+} states as well as α-Fe or α-FeO_2 due to the reactants. In the case of (3) was observed total incorporation of Fe^{3+} in the SnO_2 structure without presence of impurities.

ZnO films synthesized by thermal annealing of ZnSe/GaAs heterostructures. OLEG MAKSIMOV, Materials Research Institute, Pennsylvania State University — ZnO received much attention due to its potential application for the fabrication of ultraviolet light emitters and photodetectors. High crystalline quality films were grown using MBE, PLD, and CVD on Al_2O_3, GaN, SiC, and other substrates. However, further progress in this area is slowed down by the difficulties associated with doping ZnO p-type. Here, we report on the synthesis and doping of ZnO films using the annealing of MBE-grown ZnSe/GaAs heterostructures in the controlled environment. Se is displaced by oxygen through the reaction: 2ZnSe + 3O_2 → 2ZnO + 2SO_2. In addition, As migrating from the GaAs substrate into the ZnO layer, promotes p-type doping. While ZnGaO_2, ZnO_2, and other second phases form as the result of high temperature annealing (>700°C), stoichiometric ZnO films are obtained at moderate temperatures (~500°C). Films processed under optimized conditions exhibit sharp band edge excitations, narrow rocking curve, and are comparable with the ZnO films grown on the GaAs substrates. I would like to acknowledge support from the Office of Naval Research under grant N00014-06-1-1018.

CdTe films grown on Si, GaAs and Quartz substrates. Z.X. MA, KIN MAN YU, LBNL, LEI LIU, UCB, LAN WANG, DALE PERRY, WADEK WALKIEWICZ, LBNL, PETER YU, UC, LBNL, SAM MAO, LBNL — CdTe films of varying thickness were grown by the laser epitaxy technique on Si(001), GaAs(001), and quartz substrates. The quality of the resultant films was studied by x-ray diffraction and photoreflectance. Splitting of the valence band plus an increase in the band-gap were observed as the CdTe film thickness was decreased. To explain the observed band-gap narrowing, we would like to acknowledge support from the Office of Naval Research under grant N00014-06-1-1018.

Electrochemical capacitors and charge relaxation resistance of mesoscopic capacitors. FUMING XU, JIAN WANG, Department of Physics and the Center of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China — We investigate numerically the transport properties of a mesoscopic capacitor which consists of a quantum dot connected via a single lead to an electron reservoir. The fluctuations and distributions of electrochemical capacitance C_q and charge relaxation resistance R_q have been studied. It shows that the distribution of electrochemical capacitance C_q at one conducting channel case in our numerical calculation is different from the former theoretical prediction obtained from the scattering matrix theory. The difference is due to the existence of neutral states which has been observed in a recent optical experiment.

Porous Silicon Structures under action microwave Radiation: Charge Carrier Heating Effects. EVGENIJUS SHATKOVSKIS, JONAS GRADASAKAS, ANTANAS CESNYS, Vilnius Gediminas Technical University — Porous silicon (por-Si) is one of modern nanomaterials, which is intensively investigated recently. The action of microwave radiation is only slightly investigated on por-Si. However, basically there are papers based on application of por-Si as substrates in microwave and opto-electronic interconnects. Action microwave radiation (MW) often manifests itself through effects of charge carrier heating in semiconductors. Since the energy quanta of MW radiation are too small to challenge any quantum jumps in common semiconductors, it is likely that carrier heating can be responsible for effects arising in por-Si under MW radiation also. This question is of interest for different contributions including information storage of electrical conductivity and electroactive force (emf) in por-Si structures under the action of 10 GHz frequency MW radiation pulses. Two-terminal por-Si containing structures were made by usual technology of electrochemical etching of p-type, 0, 4 Omh cm Si plates in the HF: Ethanol=1.2 electrolyte. It has been shown that experimentally observed decrease of the resistance of the samples and rise of emf can be explained both assuming concept of hole heating, by MW radiation in fractal-like percolation grid of por-Si structure.

Magnetization of Dirac electrons in Bismuth in the quantum limit. LU LI, JOSEPH CHECK-ELSKY, Department of Physics, Princeton University, Y. HOR, R. J. CAVA, Department of Chemistry, Princeton University, C. UHER, Department of Physics, University of Michigan, NAI PHUAN ONG, Department of Physics, Princeton University — In the semimetal Bi, the Fermi Surface (FS) is comprised of 3 Dirac-like electron pockets and a hole pocket. Accurate measurements of the magnetization M in Bi were previously limited to fields B < 2 T. Following the recent report of fractional filling in Bi by Behnia et al. (Science, 2007), we have performed extensive torque magnetization measurements in fields up to 33 T, in the geometry with H at angle θ to Z (trigonal axis). At small θ, we observe a set of quantum oscillations reflecting interference between hole and electron pockets. The pattern is highly sensitive to θ. We have mapped out the variation of the periods vs. θ and H in the quantum limit (m = 1 at 9 T), and beyond. We also observe oscillations above 9 T, which correspond to fractional filling ν = 2/3 and ν = 2/5. Other anomalous features at high fields will also be reported. Resarch supported by PCCM Institute, Princeton University.
K1.00171 Variational entropy and kinetics of hot electrons\(^1\). L. MEZA-MONTES, S. BALEON, J. L. CARRILLO, Instituto de Física B. Universidad Autónoma de Puebla, Apdo. Postal J-48, Puebla, C. P. 72570, Mexico — The carrier distribution function and the effective temperature of an electronic population, optically generated in a semiconductor, are obtained by means of a variational method. An expression for the rate of entropy increment during the cooling process of the plasma is derived. We apply this expression to study the transduction processes in quantum ratchets based on resonant tunneling systems. Additionally, the relation of this rate of entropy increment to a restricted formulation of a quantum H theorem is explored.

\(^1\)Partially supported by CONACyT and VIEP-BUAP.

K1.00172 Phase switching in a voltage-biased Aharonov-Bohm interferometer. VADIM PULLER, Department of Physics, Ben-Gurion University of the Negev, Beer Sheva 84105 Israel, YIGAL MEIR, Department of Physics and The Ilse Katz Center, Ben-Gurion University of the Negev, Beer Sheva 84105 Israel — Recent experiment [Sigrist et al., Phys. Rev. Lett. 98, 036805 (2007)] reported switches between 0 and \(\pi\) in the phase of Aharonov-Bohm oscillations of the two-terminal differential conductance through a two-dot ring with increasing voltage bias. Using a simple model, where one of the dots contains multiple interacting levels, these findings are explained as a result of transport through the interferometer being dominated at different biases by quantum dot levels of different “parity” (i.e. the sign of the overlap integral between the dot state and the states in the leads). The redistribution of electron population between different levels with bias leads to the fact that the number of switching events is not necessarily equal to the number of dot levels, in analogy with experiment. For the same reason switching does not always imply that the parity of levels is strictly alternating. Lastly, it is demonstrated that the correlation between the first switching of the phase and the onset of the inelastic cotunneling, as well as the sharp (rather than gradual) change of phase when switching occurs, give reasons to think that the present interpretation of the experiment is preferable to the one based on electrostatic AB effect.

K1.00173 Study of the 2DEG in InGaAs/AlInAs heterostructures by persistent photoconductivity effect. YU-CHI HSU, C.H. HSIEH, M.H. GAU, Y.L. CHEN, W.T. CHIU, C.C. YANG, J.Y. SU, IKAI LO, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China, J.K. TSAI, Center for general education, National Formosa University, Yunlin, Taiwan, Republic of China, F.S. CHAO, Department of computer Science and Electrical Engineering, Univ. of Maryland, Baltimore, MD20742, USA — The electronic properties of the two-dimensional electron gas (2DEG) in InGaAs/AlInAs heterostructures have been studied by Shubnikov-de Haas measurement at 0.3 K. After illuminating at 0.3 K, the carrier density of the sample increased from 2.3 \(10^{12}\) cm\(^{-2}\) to 2.5 \(10^{12}\) cm\(^{-2}\) and the mobility decreased slightly from 36200 cm\(^2\)/Vs to 34000 cm\(^2\)/Vs. In order to study the effect of the channel width on the 2DEG, we made the nanometer-scaled 2DEG channels were varied with different widths of 100 nm to 500 nm. The Sdh measurement was performed on these wires for the magnetic field up to 12 T at 0.3 K. We observed the persistent photoconductivity effect on these wires and the electronic properties of these wires are under investigation.

K1.00174 Magnetotransport study on the nanometer-scaled wires made of Al\(_{1-x}\)Ga\(_x\)N/GaN heterostructures. WEN-YUAN PANG, IKAI LO, YU-CHI HSU, YEN-LIANG CHEN, MING-HONG GAU, W.S. LIN, C.H. CHEN, J.C. CHIANG, Department of physics, National Sun Yat-sen University, Kaohsiung, Taiwan, Republic of China, JEN-KAI TSAI, Center for General Education, National Formosa University, Yunlin, Taiwan, Republic of China — The electronic characteristics of nano-wires made of high-mobility Al\(_{1-x}\)Ga\(_x\)N/GaN heterostructures have been studied. The Al\(_{1-x}\)Ga\(_x\)N/GaN samples were grown on GaN-template buffer layer by plasma-assisted molecular beam epitaxy. We obtained the mobility and carrier density of two-dimensional electron gas to be 9328 cm\(^2\)/Vs and 7.91x10\(^{12}\) cm\(^{-2}\) by conventional van der pauw Hall measurement at temperature of 300 K, respectively. We prepared the samples of field-effect-transistors and reduced the width of the conducting channel from 1\(\mu\)m to 100 nm by Focus Ion Beam. The Shubnikov-de Haas oscillations were observed by magneto-resistance measurement at 0.3 K and the electronic properties for the samples of different channel widths were under investigation.

K1.00175 Transport characterization in silicon nanowires\(^3\). DIDIER STIEVENARD, IEMN - Dpt ISEN, FRANCOIS VAURETTE, BRUNO GRANDIDIER, IEMN-Dpt ISEN, DOMINIQUE DEREMES, IEMN-DptISEN, JEAN-PHILIPPE NYS, IEMN-Dpt ISEN — In spite of the great technological interest associated with nanowires, there are only few direct electrical measurements of both the doping level and of the density of surface state. Moreover, the effect of the phonon surface scattering is not well known. We have studied the transport in silicon nanowires, fabricated using e-beam lithography and RIE etching on SOI substrate (thickness of silicon : 20 nm and P-type intentionally doped at 10\(^{18}\)cm\(^{-3}\)). The nanowire widths varies from 100 nm down to 10 nm. We can extract the intrinsic resistance of the nanowires, excluding the contacts resistances. We found resistances superior to theoretical resistances. We explain these higher resistances by surface defects on nanowires naturally oxidized and we are able to determine the depletion width due to surface defects, and to deduce the doping level and the density of surface states. We found a reasonable value of 1.10\(^{13}\) to 2.10\(^{13}\) defects/cm\(^2\), associated with a doping value of 5.10\(^{19}\) to 9.10\(^{19}\) cm\(^{-3}\). Studies of the transport in the range 80 to 300 K demonstrate that the resistance of the nanowires is mainly bound to phonon scattering localized on the surface (bulk contribution is negligible).

\(^3\)We would like to thank Jacques Gautier (CEA Grenoble) for the SOI substrates.

K1.00176 Study of the Mott-insulator TiOCl under pressure and doping. YUZHONG ZHANG, ROSER VALENTI, HARALD JESCHKE, Johann Wolfgang Goethe-Universität, Institut für Theoretische Physik, S. GLAWION, M. SCHLACHTER, K. GOß, M. SCHOLZ, M. SING, R. CLAESSEN, Experimentelle Physik 4, Am Hubland, University of Würzburg, D-97074 Würzburg, Germany — We discuss recent experiments of the Mott-insulator TiOCl under pressure and Na doping in the frame of Density Functional Theory (DFT) calculations where we employ Car-Parrinello molecular dynamics with Projected Augmented Wave (PAW) wavefunctions. For TiOCl under pressure a phase transition from insulator to metal is found as observed experimentally. For the doped system we have considered supercells of Na doped TiOCl and we propose possible effective models for the mechanism of doping.

K1.00177 Quantum Optics with Colloidal Nanocrystals in Solution. DAVID BUSSIAN, LANL, ANTON MALKO, University of Texas at Dallas, YONGFEN CHEN, JENNIFER HOLLINGSWORTH, HAN HTOON, VICTOR KLIMOV, LANL — Semiconductor nanocrystal quantum dots (NQDs) have been increasingly utilized in developing technologies such as lasers, light-emitting diodes, and bioimaging. Despite gaining popularity as labeling sources in bioimaging, no reliable method has been developed to characterize and identify single nanoparticles in solution, a requirement for efficient labeling at single-cell/single-NQD level. Here we present our recent results addressing the aggregation problem by combining FCS with photon pair correlation spectroscopy (PPCS). The combination of these two methods together with necessary theoretical treatment allows us to quantify, for the first time, the clustering degree of different nanocrystals in solution. The extent of aggregation in a sample can be straightforwardly determined by the deviation of occupation number between PPCS and FCS measurements. CdSe nanocrystals dispersed in organic solvents such as toluene or hexane have minimal clustering, usually less than 1.1 NQD/cluster and do not show considerable aggregation over time. To the contrary, commercially available water-soluble CdSe NQDs that are typically used for cell labeling show a tendency toward aggregation into small, 2-3 NQD clusters. In addition, the clustering degree of such dots increases over time rendering their use in single-dot labeling problematic.
K1.00178 Energy level shift due to the co-evaporated LiF in Alq3. KINWAN PARK, HUANGJUN DING, YONGLI GAO, FRANKY SO — Recently, one of us (FS) observed strong improvement in conductivity of LiF-doped tris (8-hydroxyquinoline) aluminum (Alq3). We have investigated the p-n doping of the organic material. The doping induces energy level shift in frontier orbitals for about 0.25 eV when the doping ratio by weight is 10%. Small amount of metal deposition (0.5 % of Al, Au) on LiF-doped Alq3 causes further shift, with Al the most (∼1 eV) and Au the least (0.3 eV). Further metal depositions reverse the shift for about 0.5 eV. These results suggest that the metal induced enhancement of n-doping in LiF-Alq3 contributes to the improvement in conductivity. After 1 to 2 Å, the properties of metals show up and the Energy levels converge.

K1.00179 Discontinuity of the dielectric function at Bragg reflexes. R. HAMBACH, C. GIORGETTI, F. SOTTILE, L. REINING, LSI, CEA-CNRS UMR 7642-Ecole Polytechnique, France and ETSF France. N. HIRAOKA, Y.Q. CAI, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan. A.G. MARINOPoulos, Department of Physics and Astronomy, Vanderbilt University, Nashville, USA. F. BECHSTEEDT, IFTQ, Friedrich-Schiller Universitaet Jena, Germany. — As an example for layered materials, the loss function of graphite was studied for momentum transfers q beyond the first Brillouin zone. Surprisingly, near Bragg reflexes, the spectra are highly dependent on very small changes in q, which reminds the non-analyticity of the loss function in the optical limit (q → 0). The effect is investigated by means of first principle calculations within the random phase approximation (RPA) and is confirmed by inelastic x-ray spectroscopy (IXS) measurements. We find crystal local field effects to be crucial and propose a simple 2 × 2 model dielectric function for explanation.

K1.00180 Excitonic effects in optical absorption spectrum of CdSe/ZnSe core-shell Nanostuctures. KALUM PALANDAGE, GAYANATH FERNANDO, RAMPRI RAMPRASAD, University of Connecticut. JAMES DAVENPORT, Brookhaven National Lab — We have used a first principles, TDDFT method to study CdS (Type I) nanocrystal quantum dots and CdZnS core/shell (Type II) heteronanostructures with high accuracy. We have studied the existence of excitons and multi-excitons and the possibility of optical gain in these nanoclusters. The size dependence of the HOMO-LUMO gap, the electron-hole wave function overlap in the relevant states, coordination of atoms at the surface as well as the stability of such clusters will be presented in some detail.

K1.00181 Stark Shifts in the Mid-Infrared Absorption Edge of Type II Quantum Wells. JOHN LITTLE, KIMBERLEY OLIVER, WENDY SARNEY, STEFAN SVENSSON, Army Research Laboratory. FRED TOWNER, Maxion Technologies, QUANTUM DEVICES TEAM, MAXION TEAM — We have studied electric field induced (Stark) shifts in real-space indirect-mid-infrared transitions that occur in type II AIAs/InAs/GaSb quantum wells. Because of the spatial separation of the electron and hole wavefunctions, the potential drop between the layers dominates the shift in the absorption edge, and can result in either a red shift or a blue shift, depending on the ordering of the quantum wells within the intrinsic region of a p-n diode. Of particular interest is the case in which a reverse bias on the diode yields a blue shift in the absorption edge since this field tends to increase the overlap between the electron and hole wavefunctions, increasing the absorption strength. We will give the results of low temperature photocurrent spectroscopy on a series of samples with different layer ordering, degrees of confinement, and coupling between the wells.

K1.00182 Reflectance anisotropy spectroscopy of II-VI semiconductor surfaces. R. A. VAZQUEZ-NAVA, N. ARZATE, B. S. MENDOZA, Centro de Investigaciones en Optica — The spectroscopical reflectance anisotropy (RA) response of II-VI semiconductor surfaces, which exhibits different reconstructions are studied. We use, an ab initio pseudopotential calculation in the framework of the density functional theory and within the local density approximation (DFT-LDA) to obtain the relaxed atomic positions, and then we use a microscopic formulation based on a semi-empirical tight binding (SETB) approach which includes spin-orbit (SO) interactions[1] to obtain the RA spectra. We show RA spectrum of each surface reconstruction and compare our theoretical results with experimental. We find a good agreement between experimental and theoretical spectra.[1] R.A. Vázquez-Nava, B.S. Mendoza and C. Castillo, Phys. Rev. B 70, 165306 (2004).

K1.00183 Ultrafast nonlinear spectroscopy characterization of CdSe quantum dots. QIGUANG XU, SHENGMIN MA, BACHER TABIBI, JAETAE SEO, Hampton University. WILLIAM YU, Worcester Polytechnic Institute. HAMPTON UNIVERSITY COLLABORATION, WORCESTER POLYTECHNIC INSTITUTE COLLABORATION — Frequency degenerate and nondegenerate two-photon absorption spectra of direct band gap semiconductor quantum dot samples, such as CdSe and CdTe, have attracted great attention recently because of their potential applications in nonlinear photonic devices. In this work, we used the femtosecond time-resolved photon echo technique to characterize the third-order nonlinear optical properties of CdSe quantum dots in toluene. The quantum dots had an average size of about 3 nm and the lowest absorption peak at 559 nm. A femtosecond laser with 150 fs pulsewidth and 1 kHz repetition rate was used for the measurement. The copolarization hyperpolarizability at 775 nm was found to be about 1 x 10^-14 m^2/V^2 and the dephase time was shorter than the resolution limitation of our system at room temperature. This work at Hampton University was supported by Army Research Office (W911NF-07-1-0608) and National Science Foundation (HRD-074635, HRD-0630372, ESI-0426328/002, and EEC-0532472).

K1.00184 Direct bandgap of group IV semiconductors by uni-axial stress. FENG ZHANG, Department of Physics, Penn State University. PEIHONG ZHANG, Department of Physics, SUNY at Buffalo. VINCENT CRESPI — We theoretically examine the possibility of converting typical group IV semiconductors Si, SiGe (zinc blende), and Ge into direct bandgap materials by uniaxial stress along the (111)> and (100) directions. For silicon, the required tensile strain is too large to be practical. For SiGe and Ge along [111], the conduction band splitting at the L point lowers the required longitudinal strain along [111] to 7%. For SiGe, the required strain along [111] is 3% and 4% for GeSi and Ge, respectively. For Ge along [100], the position of the conduction band edge at the Γ point varies sub-linearly with strain; therefore strain along [100] is less efficient: GeSi is unlikely to achieve a direct gap by extension along [100] and Ge requires a 6% longitudinal strain. The full dependence of the indirect/direct transition on arbitrary combinations of uniaxial/hydrostatic tensile strain is given for both GeSi and Ge.

K1.00185 Quasi-particle spectra of various forms of crystalline Germanium Telluride. JINWOO KIM, Department of Physics, Pohang University of Science and Technology. GEUNSIK LEE, Department of Physics, University of Texas at Dallas. SEUNGHOO JHI, Department of Physics, Pohang University of Science and Technology — GeTe is known to undergo a very complex structural phase transition under pressure. Also it changes the phase upon heating from crystalline NaCl structure to amorphous phase. Several models were suggested for possible structural transition pathways such as Toledano, Modified Buerger and Watanabe model. We have investigated the dielectric function of GeTe at representative structural phases using the pseudopotential density functional method within the generalized gradient approximation. To calculate the quasiparticle spectra, we carried out the GW calculations. Semicore d-electrons of Te are found to be very critical for calculating correct transition pressures, and they are included explicitly as valence. These electrons affect the electronic structures through the p-d coupling, which is found non-negligible. Our results can help analyze experimental data and investigate the transition pathway of GeTe.
K1.00186 Spectroscopic characterization of Europium and Praseodymium doped Gallium Nitride powders. E. I. BROWN, OLUSOLA OYEBOOLA, UWE HOMMERICH, Hampton University, TAKAHIRO YAMADA, HIROSHI NABU, HISANORI YAMANE. Tohoku University, KENJI KOHIRO, YOSHIKO TSUCHIDA, Tsukuba Research Laboratory, JOHN ZAVADA, US Army Research Office — Rare earth (RE) doped GaN continues to be of interest for applications in display technology, solid-state light sources, and optical communications. Recently, RE doped GaN powders have been prepared using different methods including flux techniques and combustion synthesis. In this work, we report on the luminescent properties of Eu$^{3+}$ and Pr$^{3+}$ doped GaN powder prepared by a Na flux method for potential applications in light source development. Under above-gap pumping, GaN:Eu and GaN:Pr powders exhibited intense red emissions at $\sim$621 nm and $\sim$652 nm, which corresponds to the intra-4f RE$^{3+}$ transitions $^7$D$_0$ $\rightarrow$ $^7$F$_2$ and $^3$P$_0$ $\rightarrow$ $^3$F$_2$ states, respectively. A temperature dependent study of the red emission showed that the integrated PL intensity is quenched at room-temperature by $\sim$30% and $\sim$50% for Pr:GaN and Eu:GaN, respectively. More results of temperature dependent and time-resolved emission spectroscopy of Eu and Pr doped GaN powders will be presented at the conference.

K1.00187 Electronic structure and conduction-band mass of InN under pressure. NIELS E. CHRIS- TENSEN, Dept. of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus, Denmark, IZA GORCZYCA, Inst. of High Pressure Physics, Polish Academy of Sciences, Warsaw, AXEL SVANE, Dept. of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus C, Denmark — An initio calculations for n-type InN of the band structure and effective masses (optical- and curvature-) in the lowest conduction band as functions of applied pressure and varying electron concentration are presented. The calculations as well available experimental data demonstrate the strong non-parabolicity of the InN conduction band.

K1.00188 Temperature dependence of the InGaPN conduction band structure. K. L. LIN, T. S. WANG, J. S. HWANG — Material properties of III-N-V alloys, such as GaAsN, InGaAsN, and InGaPN, have been intensively studied, because a small amount of nitrogen (N) incorporation results in very large bandgap bowing and dramatic change in the band structure.1,2 Recently, temperature dependence of the parameters, i.e. the localized states energy $E_N$ introduced by an isolated N and the interaction potential $V$, of the band anticrossing (BAC) model in GaAsN epilayers has been reported.3 These properties have never been studied for InGaPN. In this work, temperature-dependent photoreflectance (PR) measurements are employed to characterize the conduction band structure of In$_{0.54}$Ga$_{0.46}$P$_1-y$N$_y$ ($y = 0$ and 0.02) grown on GaAs substrates. The band gap and the upper subband $E_+$ are observed in InGaPN as predicted by the BAC model. To investigate the energetic positions of the features in the PR spectra, a Kramers-Kronig analysis is proposed. Based on these PR data and the BAC model, we find $E_N$ = 2.054 eV and $V = 1.513$ eV at 293 K. With decreasing temperature, the energy of $E_N$ shifts significantly to higher energies. Simultaneously, the interaction potential $V$ between the N states and the host conduction band also rises to higher values. The thermal shifts of $E_N$ and $V$ are $dE_N/dT \approx -0.43$ meV/K and $dV/dT \approx -0.67$ meV/K, respectively. 1. APL 88, 031907 (2006). 2. APL 89, 192116 (2006). 3. APL 89, 202105 (2006).

K1.00189 Electron pairing in small Hubbard Clusters. KALUM PALANDAGE, GAYANATH FERNANDO, University of Connecticut, ARMEN KOCHARIAN, California State University, JAMES DAVENPORT, Brookhaven National Lab — Exact thermal studies of 4-site Hubbard Nanoclusters are carried out using the analytical eigenvalues. Electron pairing is seen when the on-site Coulomb interaction is smaller than a critical value Uc(T) in the repulsive Hubbard clusters which also show spin pairing at a lower temperature. Specific heat and probability calculations provide strong support for the existence of competing (paired and unpaired) phases near optimal doping. Attractive 4-site Hubbard model can be mapped on to the repulsive model and these studies can be used to understand ferroelectricity in certain metal clusters.

K1.00190 Dipole model for Non linear response of adsorbed overlayers1. R. A. VAQUEZ-NAVA, N. ARZATE, Centro de Investigaciones en Optica, J. E. MEJIA, Centro Universitario de los Lagos, U de G. Mexico, W. L. MOCHAN, Instituto de Ciencias Fisicas, UNAM, Mexico — We present theoretical calculations of second harmonic generation (SHG) from overlayers of alkali atoms adsorbed on a crystalline metallic surface. We assume that the overlay is formed by an ordered two-dimensional (2D) array of adatoms that respond to the local electric field like point-like harmonic oscillators. We consider overlayers with several rational coverages, assuming that the adsorbates occupy high symmetry sites which form a Bravais lattice that is commensurate with the substrate [1,2]. SHG spectra are obtained for the five 2D Bravais lattices. We found that SHG can be used to observe ordered phases when the ordered phase has a rectangular, centered-rectangular or oblique symmetry. [1] H. Arce, W. L. Mochan and G. Cocho, Surf. Sci. 294, 108 (1993). [2] H. Arce and W. L. Mochan, J. Phys.: Condens. Matter 5, A101 (1993).

K1.00191 Magneto-exciton transitions in laterally coupled quantum dots1. ZDENKA BARTEVIC, MONICA PACHECO, Depto. de Fisica, Universidad Tecnica Federico Santa Maria, CARLOS A. DUQUE, Instituto de Fisica, Universidad de Antioquia, LUIZ E. OLIVEIRA, Instituto de Fisica, Universidade Estadual de Campinas - UNICAMP — We present a study of the electronic and optical properties of laterally coupled quantum dots. The excitonic spectra of this system under the effects of an external magnetic field applied perpendicular to the plane of the dots is obtained, with the potential of every individual dot taken as the superposition of a quantum well potential along the axial direction with a lateral parabolic confinement potential, and the coupled two- dot system then modeled by a superposition of the potentials of each dot, with their minima at different positions and truncated at the intersection plane. The wave functions and eigenvalues are obtained in the effective-mass approximation by using an extended variational approach in which the magneto- exciton states are simultaneously obtained [1]. The allowed magneto-exciton transitions are investigated by using circularly polarized radiation in the plane perpendicular to the magnetic field. We present results on the excitonic absorption coefficient as a function of the photon energy for different geometric quantum-dot confinement and magnetic-field values. Reference: [1] Z. Barticic, M. Pacheco, C. A. Duque and L. E. Oliveira, Phys. Rev. B 68, 073132 (2003).

K1.00192 Anisotropy of plasmon spectrum due to joint Rashba and Dresselhaus spin-orbit interaction1. SAMVEL BADALYAN, Department of Radiophysics, Yerevan State University, 375025 Armenia and Department of Physics, University of Regensburg, 93040 Regensburg, Germany, ALEX MATOS-ABIAGUE, Department of Physics, University of Regensburg, 93040 Regensburg, Germany, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri - Columbia, Missouri 65211, USA, JOARSLAV FABIAN, Department of Physics, University of Regensburg, 93040 Regensburg, Germany — We have investigated the combined effect of Rashba and Dresselhaus spin-orbit interaction (SOI) on the many-body polarization function of a two-dimensional electron system (2DES). The dielectric function of a 2DES is calculated within the random phase approximation and the plasmon energy spectrum as a function of the momentum magnitude for its different orientations is obtained. Our calculations show the peaked behavior of dynamical structure factor as a function of the polar angle of momentum. This strong peak corresponds to the plasmon, which is damped due to SOI. Thus, we have clearly demonstrated that due to the anisotropy of the spin-orbit interaction, the plasmons with the definite values of energy and momentum can be excited only in the certain direction.

1This work is supported by the Volkswagen Foundation, the DFG Grant Sonderforschungsbereich 689, and NSF Grant No. DMR-0313681.
K1.00193 A STM study on temperature-dependent adsorption of H₂O on Si(001)  
SANG-YONG YU, HANCHUL KIM, JA-YONG KOO, KRIS, KRIS TEAM — We studied the temperature dependence of water molecule adsorption on the Si(001)-2×1 surface by using Scanning Tunneling Microscopy. The water molecules are known to dissociate during the adsorption on Si(001) and form Si-H and Si-OH bonds. Recently, we demonstrated that they are two adsorption configurations: ID (inter-dimer) and OD (on-dimer). These two configurations show population ratio of n(ID)/n(OD) ~ 5 at Room Temperature. In order to understand the adsorption kinetics more thoroughly, we have measured n(ID)/n(OD) by varying the sample temperature from 300K to 870K. It is found that n(ID)/n(OD) show strong temperature dependence, and it even becomes smaller than 1. The cross-over temperature is at around 470K.

K1.00194 Phase Transition Plasticity Response in Uniaxially Compressed Silicon Nanospheres  
TRAIAN DUMITRICA, PAOLO VALENTINI, Department of Mechanical Engineering, University of Minnesota, WILLIAM W. GERBERICH, Department of Chemical Engineering and Materials Science, University of Minnesota — We present a microscopic description for the response of crystalline Si nanospheres up to 10 nm in radius for various uniaxial compression levels. The behavior at low compressions closely resembles the Hertzian predictions. At higher compressions the creation of a new beta-tin phase in the particle core leads to (i) volumetric changes (ii) an increase in elastic moduli, and (iii) significant hardening. Further, (iv) a reversible character of the transformation is obtained with molecular dynamics simulations. The agreement of (i)-(iv) with recent experimental findings [1] challenges the current exclusive view of a dislocation plasticity response in somewhat larger nanoparticles. The phase transition path should dominate in ultrasmall structures, where dislocation activity is prohibited. [1] W. W. Gerberich et al., J. Mech. Phys. Sol. 51, 979 (2003).

K1.00195 Friction measurements on InAs NWs by AFM manipulation  
HAKAN PETTERSSON, Halmstad University, Halmstad, Sweden, GABRIELA CONACHE, Halmstad University, Halmstad, Sweden, STRUAN GRAY, Lund University, Lund, Sweden, MICHAEL BORDAG, Leipzig University, Leipzig, Germany, ALINE RIBAYROL, LINUS FROBERG, LARS SAMUELSON, LARS MONTELIUS, Lund University, Lund, Sweden — We discuss a new approach to measure the friction force between elastically deformed nanowires and a surface. The wires are bent, using an AFM, into an equilibrium shape determined by elastic restoring forces within the wire and friction between the wire and the surface. From measurements of the radius of curvature of the bent wires, elasticity theory allows the friction force per unit length to be calculated. We have studied friction properties of InAs nanowires deposited on SiO₂, silanized SiO₂ and Si₃N₄ substrates. The wires were typically from 0.5 to a few microns long, with diameters varying between 20 and 80 nm. Manipulation is done in a ‘Retrace Lift’ mode, where feedback is turned off for the reverse scan and the tip follows a nominal path. The effective manipulation force during the reverse scan can be changed by varying an offset in the height of the tip over the surface. We will report on interesting static- and sliding friction experiments with nanowires on the different substrates, including how the friction force per unit length varies with the diameter of the wires.

K1.00196 First-Principles Theoretical Analysis of Dopant Diffusion on Surfaces of II-VI Compound Semiconductor Nanocrystals  
TEJINDER SINGH, T.J. MOUNTZIARIS, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present a detailed analysis of diffusion of dopants (e.g., Mn, Cu) on surfaces of ZnSe nanocrystals and discuss its implications for dopant incorporation into the growing nanocrystals. We focus on nanocrystals with diameters d ~ 5 nm that have polyhedral shapes with well-defined facets. Using first-principles density functional theory calculations, we have studied the dopant diffusion and adsorption mechanisms and obtained the energetics of various possible dopant diffusion pathways. ZnSe(001)-2×1 is found to be the energetically favorable surface for dopant binding, with multiple adsorption sites. Our results indicate that dopant atoms can migrate with low activation barriers along the Se dimer rows without substantial surface relaxation. Diffusion across the dimer rows is governed by a higher-barrier pathway, which can lead to dopant incorporation into the nanocrystal through strong bonding with the nanocrystal surface at the corresponding adsorption site in the trough between adjacent dimer rows.

K1.00197 Structural defects in SiC nanowires  
RENBING WU, FENG LIU, Department of Materials Science and Engineering, Zhejiang University — High-resolution transmission electron microscopy (HRTEM) and selected area electron diffraction (SAED) are used to investigate structural defects in zinc blende SiC nanowires produced by a vapor-solid (VS) mechanism. It is found that the defects exist as the stacking faults and twins including single twin, double twins, and quasiperiodic placement twins. The results indicate that the important role of defects in determining the morphologies and structures i.e. stacking faults result in formation of branches or junctions, while twins cause kinks, bamboo or a zigzag appearance. Based on the characterizations, the defects formation mechanism and the influence on the nanowire growth kinetics and behavior are also discussed.

K1.00198 Nonlinear modification of tunneling and conductivity in two-dimensional electron gas–impurity system in strong high-frequency electric fields  
DMITRY SOLENOV, VLADIMIR PRIVMAN, Department of Physics, Clarkson University, Potsdam, New York 13699-5820 — We investigate two-dimensional electron gas system coupled to adjacent impurity sites. When a high-frequency uniform electric field is applied perpendicular to the electron gas layer it significantly modifies electron correlations in the impurity–gas system. At strong magnitudes of external field the system enters nonlinear dynamical control regime, similar to double quantum dot structures. In contrast to the latter, coulomb activation of the impurity sites introduces strong scattering for conduction electrons that leads to nontrivial renormalization of the tunneling. Modification of tunneling rates as a function of the field amplitude is calculated. We show that for low enough temperatures this effect is manifested in nonlinear modification of tunneling and conductivity in two-dimensional electron gas–impurity system in strong high-frequency electric fields.

K1.00199 Influence of inactivated dopants clusters and post annealing on electrical and optical properties of indium tin oxide on plastic substrates  
TERRY ALFORD, HAUK HAN, School of Materials and Flexible Display Center at Arizona State University, JAY LEWIS, Center for Materials and Electronic Technologies, RTI International — Indium tin oxide (ITO) films have been introduced as a transparent electrode for large area electronics such like display and photovoltaics due to their high electrical conductivity coupled with high transmission. This study describes the influence of Sn defect clusters on the electrical and optical properties of the ITO films. Absorption coefficient analysis indicates that electrically inactive Sn clusters generate defect states within the band gap and strongly affect the electrical and optical properties of the ITO films. Electrical and optical properties of ITO films are enhanced by reduction of Sn defect clusters with activation of Sn dopants, upon heat treatment. To explain the enhanced carrier transport property, we propose the reaction model based on our Rutherford backscattering spectrometry (RBS), Hall measurement, and x-ray photoelectron spectroscopy (XPS) data. The proposed model describes Sn⁴⁺ ions forming a neutral defect complex with Sn⁵⁺ ions which may not contribute to electrical conductivity in the amorphous phase. These Sn defect clusters in the amorphous phase dissociate and could contribute to an increase in Sn⁴⁺ concentration in ITO films without changing oxygen contents.
**K1.00200** Hole mobility in Copper-doped CdTe films. Z.X. MA, KIN MAN YU, LBNL, LEI LIU, LBNL, UCB, LAN WANG, DALE PERRY, WALDEK WALUKIEWICZ, LBNL, PETER YU, UCB, LBNL, SAM MAO, LBNL — Copper-doped CdTe films have been grown by the laser epaaxy technique. X-ray diffraction, Rutherford backscattering, and photoflectance spectroscopy were utilized to characterize the CdTe/Cu films. Structural analysis suggests that the growth of CdTe/Cu on GaAs(100) is initiated along the (100) orientation, but changes to the (111) direction after the film thickness exceeds 400 nm. Hall effect measurements indicate that copper doping can achieve hole mobility over 150 cm²/Vs at room temperature. Changes in the hole effective mass and phonon spectra have been calculated to explain the enhanced hole mobility in Cu:CdTe.

1Supported by the U.S. Department of Energy, NNSS/NA-22, under contract No. DE-AC02-05CH11231.

**K1.00201** An experimental study on $\Gamma(2)$ modular symmetry in the quantum Hall system with a small spin-splitting, C.F. HUANG, CMS/ITRI, Y.H. CHANG, Dept. of Physics, NTU, H.H. CHENG, Z.P. YANG, Center for Condensed Matter Sciences, NTU, H.D. YEH, CMS/ITRI, C.H. HSU, C.-T. LIANG, Dept. of Physics, NTU, D.R. HANG, Dept. of Materials Science and Optoelectronic Engr., Natl. Sun Yat-sen Univ., H.H. LIN, Dept. of Elec. Engr., NTU — Magnetic-field-induced phase transitions are investigated by performing transport measurements on the two-dimensional (2D) electron system in an AlGaAs/GaAs heterostructure at low temperatures. [1] Both the semicircle law and universal two-parameter scaling are observed as the spin-splitting becomes resolved with increasing the magnetic field $B$ perpendicular to such a 2D system. The critical resistivities, however, are not of the expected universal values, and the modular symmetry is reduced from $\Gamma_0(2)$ to $\Gamma(2)$. On the other hand, $\Gamma_1(2)$ symmetry survives at lower $B$ where the spin-splitting is unresolved. Therefore, the reduction of the modular symmetry can be due to the resolved small spin-splitting as predicted by Dolan [2]. Such a small splitting not only reduces the modular symmetry, but also breaks the scaling on the longitudinal conductivity $\sigma_{xx}$ at higher temperatures. It is found that the scaling on the Hall conductivity $\sigma_{xy}$ is more robust than that on $\sigma_{xx}$ under a small spin gap. References [1] C. F. Huang, Y. H. Chang, H. H. Cheng, Z. P. Yang, H. D. Yeh, C. H. Hsu, C.-T. Liang, H. H. Lin, D. R. Hang, and H. H. Lin, J. Phys. Condens. Matt. 19, 026205 (2007).


**K1.00202** Probing insulator-quantum Hall transitions near the onset of Landau quantization in GaAs/AlGaAs heterostructures, KUANG YAO CHEN, National Taiwan University, Y.H. CHANG, C.-T. LIANG, National Taiwan University, N. AOKI, Y. OCHIAI, Chiba University, CHUN FENG HUANG, NML/CMS ITRI, LI-HUNG LIN, National Chiao Tung University, K. A. CHENG, Lung-Hwa University of Science and Technology, H.H. CHENG, H.H. LIN, National Taiwan University, JAU-YANG WU, SHENG-DI LIN, National Chiao Tung University — Magneto-transport measurements are performed on the two-dimensional GaAs electron systems (2DESs) to study the low-field insulator (I) and quantum Hall (QH) effect. With increasing the perpendicular magnetic field $B$, the 2DESs undergo direct I-QH transitions to enter QH liquids from the low-field insulators.


**K1.00203** Single-valley (110) and double-valley (001) AlAs quantum wells, DASGUPTA, A. FONTCUBERTA, M. BICHLER, G. ABSTREITER, Walter Schottky Institute, TU Munich, Germany, M. GRAYSON, Walter Schottky Institute, TU Munich, Germany & Dept. of Electrical Engineering and Computer Science, Northwestern University — Doubly-degenerate valley quantum number in (001)AlAs quantum wells (QWs) functions as pseudo-spin degree of freedom for understanding exchange interactions, and single valley anisotropic mass, if observed in high mobility (100)AlAs, could lead to interesting phases in quantum limit. We optimized growth of AlAs QWs [1], and grew (001) oriented double valley degenerate AlAs QW with density $n=2.4 \times 10^{11}$ cm$^{-2}$ and mobility $\mu=4.3 \times 10^2$ cm$^2$/Vs (330 mK), an improvement of almost an order of magnitude over published results. We also grew (110)oriented AlAs QW with $n=4.2 \times 10^{11}$ cm$^{-2}$ and $\mu=5.4 \times 10^4$ cm$^2$/Vs (330 mK). The (110)AlAs QW is predicted to occupy single valley, and anisotropic $\mu$ along two crystallographic directions of (100) & (1-10) may be expected. Experimentally, we observed $\mu$ anisotropy $\mu_{(100)}/\mu_{(1-10)}=1.5$ in dark (1.4 K) and strong odd-filling factor $S$Doh gaps, evidence consistent with single valley occupancy. We studied $\mu$ on both growth facets as function of temperature. The $\mu$ of (110)AlAs QWs is seen to saturates below the Fermi temperature but (001)AlAs QW does not saturate.

**K1.00204** ABSTRACT WITHDRAWN —

**K1.00205** Analysis of spin current shot noise from a quantum dot coupled to a quantized bosonic field, MARKO ZIVKOVIC, IVANA DJURIC, CHRISTOPHER SEARCH, Department of Physics and Engineering Physics, Stevens Institute of Technology, Castle Point on Hudson, Hoboken, NJ 07030 — We examine spin current generated by quantum dots coupled to quantized bosonic field. The dots are connected to normal leads at zero bias voltage across the dot. We model the dot as a two level spin system with one of the spin states lying below the Fermi level of the leads and the other above. Spin flips followed by subsequent tunnelling out into the leads generate a pure spin current in the absence of any charge current. The dot is coupled to a quantized bosonic field that influences the generation of spin current in one of two possible scenarios. First, we consider spin flips induced via Raman transitions in optical microcavity. Secondly, electron spin resonance via classical magnetic field induces spin flips in the presence of a quantized phonon field that modulates the energy levels of the dot. In the limit of strong Coulomb blockade our model is analogous to the Jaynes-Cummings model in quantum optics. In the case of optical cavity mediated spin flips, we show that the spin current is bistable for a coherently driven cavity and this bistability is clearly visible in the spin current shot noise. A comparison of spin current and shot noise for interactions with different bosonic fields is presented.

**K1.00206** Magneto-Dynamics of a Double Quantum Dot System, N.J.M. HORING, D. MIESSEIN, Stevens Inst. of Tech., L.Y. CHEN, University of Texas at San Antonio, QEPT TEAM — We have examined the microscopic dynamics of a double quantum dot system modeled by a potential having two three-dimensional Dirac functions of generally unequal strengths separated in position by $\vec{r}$:

$$V(\vec{r}) = -\alpha_1 \delta^{(3)}(\vec{r} - \vec{d}/2) - \alpha_2 \delta^{(3)}(\vec{r} + \vec{d}/2).$$

While these delta function potentials individually support a single energy level, the introduction of a strong magnetic field gives rise to Landau quantization and a plethora of energy levels. The relative magnitude of $\alpha_1/\alpha_2$ affects the bonding/antibonding character of the states, as well as the multiplicity of levels induced by magnetic quantization.
K1.00207 Magnetotransport Properties of Ferromagnetic Semiconducting Fe1−xCo2Si Alloy Nanowires: Building Blocks for Silicon Based Spintronics, SONG JIN, University of Wisconsin-Madison. Fe1−xCo2Si alloys were recently shown to be concentrated magnetic semiconductors and can be promising materials for spin injection into silicon not only because of its high spin polarization but also because of its CMOS compatibility. By developing a rational approach to synthesizing nanowires using single source precursors, we have realized a host of new transition metal silicide nanowires through chemical vapor deposition/transport. We have synthesized FeSi nanowires using Fe(SiCl3)2(CO)4 and CoSi nanowires using Co(SiCl3)(CO)4. Building on these initial successes, we synthesized magnetic semiconducting Fe1−xCo2Si alloys using mixed precursors. The as synthesized nanowires were characterized using high resolution transmission electron microscopy, energy dispersive X-ray spectroscopy, and X-ray absorption spectroscopy. The bulk Fe1−xCo2Si alloys were recently shown to be concentrated magnetic semiconductors and can be suitable materials for spin injection into silicon because of its CMOS compatibility. The interesting magnetic semiconducting behavior is shown using magnetotransport and X-ray magnetic circular dichroism revealing the interesting chemistry behind the magnetic properties. These novel magnetic semiconducting silicide nanowires are exploited as building blocks for silicon-based spintronic nanodevices.

K1.00208 Adsorption, Symmetry and Magnetic Properties in TM-GaN Nanocrystals, HE YAN DONG, KEMING FU, MING JIANG, Dept. of Physics, Yantai University, P.R. China. — Transition metal(TM)-doped dilute magnetic semiconductor nanocrystals are of interest for potential applications in spintronics due to their tunable properties. The interest of semiconductor nanocrystals depend on their size or shape, we present first-principles calculations for the electronic structure and magnetic properties of completely passivated, H-adSORBED and isolated Mn/Co-doped GaN nanocrystals with different point symmetry. A novel half-metallicity and magnetic metastability has been found. The multiple metastable spin states and spin-flip for metallic channel are demonstrated in these nanocrystals with the various H coverages and point groups symmetry. A detailed electronic structure analysis is given. Our calculated results imply a new type of half-metallic and spin-crossover nanomaterial.

K1.00209 Ab Initio Study of Magnetic Properties of Cr-doped Chalcopyrites: (BeSn, BeGe, MgGe)N2, J. RUFINUS, Widener University, Chester, PA 19013. J. L. DEWINTER, California Polytechnic State University, San Luis Obispo, CA 93407, — A Density Functional Theory within Generalized Gradient Approximation study of three thermodynamically stable Cr-doped (II-IV)-V2 chalcopyrites: (BeSn, BeGe, MgGe)N2 was performed. Since the chalcopyrites are ternary materials, there are possibilities of having ferromagnetic or antiferromagnetic configurations, depending on which metal was substituted by the dopant. The results show both BeSnN2 and BeGeN2 to be ferromagnetic independent of the substitution sites. On the other hand, MgGeN2 was found to be antiferromagnetic for CrAlP (Cr substitutes Mg site) and ferromagnetic for CrGe (Cr substitutes Ge site.)

1Work supported by the NSF (Grant number ECS-0609129)

K1.00210 Electron spin splitting effect in AlSb/InAs/AlSb quantum wells, MINUKIM, TAKAKIKOGA, Faculty of Engineering and Graduate School of Information Science and Technology, JUSST, Research Institute of Electrical Communication, Tohoku Univ., Japan. — We investigated the electron spin splitting effect in AlSb/InAs/AlSb quantum wells (QW) both experimentally and theoretically. Our experiment was performed on MBE grown high quality AlSb/InAs/AlSb QW samples with Mn potential symmetry was controlled by intentional/unintentional dopings near the QW layer, where we didn’t observe the beating pattern in the Shubnikov de Haas (SdH) oscillations experimentally. Although the presence of the beating pattern in the SdH oscillations can be considered as a side-evidence of the zero-field spin splitting in the pertinent 2DEG (two dimensional electron gas), the absence of it does not necessarily support the absence of the zero-field spin splitting. Our theoretical analysis including all the Rashba, Dresselhaus and Zeeman spin-splitting Hamiltonians revealed that the absence of the SdH oscillations itself is not inconsistent with the presence of the zero-field spin splitting in our specific samples. Considering the fact that SdH oscillations itself are not necessarily support the absence of the zero-field spin splitting.

K1.00211 Low-temperature spin dynamics of Mn-rich Mn(Ga)As nanoclusters embedded in a GaAs matrix, WEIZHU WANG, JIAJUN DENG, JUN LU, BAOQUAN SUN, JIANHUA ZHAO, State Key Laboratory for Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences — Recently, the composite systems of Mn-rich Mn(Ga)As nanoclusters embedded in GaAs matrices have received an increasing attention due to the large magneto-optical and magneto-resistance effects at room temperature which could be applied to spin-electronic devices. In this work, we report the low-temperature spin dynamic behaviours including memory effects and slow magnetic relaxation of such composite systems. The systems can be formed by in situ postgrowth annealing of (Ga,Mn)As films at 650 °C for 10 min because of spinodal decomposition. High-resolution TEM images show zincblende Mn-rich Mn(Ga)As nanoclusters with a diameter in the range of 10-20 nm embedded in a GaAs matrix. From zero-field cooled and field cooled measurements, we can observe a clear bifurcation of the two curves demonstrating the existence of the spin-glass-like phase below the blocking temperature in the systems with high Mn concentration. Memory effects and slow magnetic relaxation, the typical characteristics of spin-glass-like phases, are also detected, and the hierarchical model is confirmed to be in accordance with such low-temperature behaviours. On the other hand, for samples with low Mn content, ferromagnetic order remains up to 360K.

K1.00212 Proposal of Spin Interference Experiment Using GaAs/AlGaAs Heterostructures, KAZUAKI NISHIO, LI ZHANG, TAKAAKI KOGA, GSIST and CRIS (SOUSEI), Hokkaido University, Sapporo, Japan, and TOSHIYUKI KOBAYASHI, TATSUSHI AKAZAKI, NTT BRL, NTT Corporation, Atsugi, Japan. — We propose a spin interference (SI) experiment [1] using GaAs/AlGaAs system, where the zero-field spin-splitting (Δ0) is caused by the Dresselhaus term predominantly. GaAs/AlGaAs has the advantage in gating stability and long carrier mean free path relative to the other III-V materials, making it a standard semiconductor in mesoscopic physics experiment. It is shown theoretically as well as experimentally that values of Δ0 are generally smaller in GaAs/AlGaAs than in InGaAs/InAlAs. In the present work, however, we suggest that the gate-controllability of spins in GaAs/AlGaAs, Δ0 ≈ Δ0/h, being the relevant parameter, should also be as good as that in InGaAs/InAlAs based on our simulations, which makes the SI experiment possible even with GaAs/AlGaAs. We fabricated a series of quantum nanowires on GaAs/AlGaAs wafers with various wire widths. We discuss their transport properties and the prospective for the future SI experiment. [1] Koga et al., PRB 70, 161302(R) (2004); ibid. 74, 041302(R) (2006)

1also with CREST, JST.
K1.00213 Electrical spin injection and detection by ballistic transport in MnAs / GaAs : MnAs spin–valve hybrid heterostructures. PHAM NAM HAI, YUSUKE SAKATA, MASAFUMI YOKOYAMA, Dep. of Electronic Eng., The Univ. of Tokyo, SHINOBU OHYA, MASAaki TANAKA, Dep. of Electronic Eng., The Univ. of Tokyo; JST — Electrical spin injection and detection by ballistic transport of spin-polarized carriers in ferromagnet (FM) / semiconductor (SC) / ferromagnet (FM) hybrid structures are key issues in semiconductor-based spintronics. By using ballistic transport of spin-polarized carriers, we can improve the spin injection / detection efficiency without using a high tunnel barrier at the FM/SC interface that decreases the current driving capability when used in active devices. In this paper, we report on the spin injection and detection by ballistic transport in perpendicular spin-valve hybrid heterostructures consisting of MnAs (20 nm) / GaAs (10 – 30 nm) / GaAs: MnAs (5 nm) grown by molecular beam epitaxy. The GaAs:MnAs layer contains ferromagnetic MnAs nanoclusters embedded in a GaAs matrix, and acts as a spin injector and a spin detector. Several % of spin-valve MR ratio was clearly observed up to 300 mV at temperature lower than 90 K. Considering the fact that all the junctions showed ohmic current-voltage characteristics, the spin-valve MR would be 10^{-6} for purely diffusive transport regime. Consequently, the spin-valve MR signal of several % is caused by the ballistic transport of spin-polarized carriers in the GaAs layer.

K1.00214 Observation of intrinsic spin-Hall effect in transport. EWELINA HANKIEWICZ, Fordham University, MARKUS KOENIG, ALENA NOVIK, Wuerzburg University, JAIRO SINtOVA, Texas A&M University, HARTMUT BtHMANN, LAURENS MOLENKAMP, Wuerzburg University — We study spin transport in n and p-doped mesoscopic H-bar structures fabricated from HgTe/HgCdTe quantum wells. In experiment the current is driven in one leg of H-bar structure while the second one is used to detect the voltage signal (similar to proposal presented in PRB 70, 241301(2004)). In p-doped samples, our data seem to confirm the existence of intrinsic spin-Hall effect. We also present the Landauer-Buttiker calculations with realistic parameters and details of band structure to verify experimental observation.

K1.00215 SOCIETY OF PHYSICS STUDENTS —

K1.00216 Crystal Growth of Quasi-One Dimensional SrNbO$_3$ and LaTiO$_3$$_{3,41}$. ANN DEML, University of Wisconsin-River Falls, C. A. M. DOS SANTOS, Escola de Engenharia de Lorena-USP, JOHN NEUMEIER, B. D. WHITE, Montana State University — Single crystals of SrNbO$_3$$_{4,1}$ and LaTiO$_3$$_{3,41}$ were grown in order to investigate the physical properties of these quasi-one dimensional conductors. Single crystals growth was accomplished with an optical image furnace; the synthesis was performed with X-ray powder diffraction. The resistivity and heat capacity of SrNbO$_3$$_{4,1}$ were measured in the temperature range 300 K $>$ T $>$ 0.3 K. SrNbO$_3$$_{4,1}$ was annealed to examine the influence of oxygen content on the electrical resistivity. The Debeye temperature and heat capacity coefficient of SrNbO$_3$$_{4,1}$ were found to be 458.5 $\pm$ 0.2 K and 0.77 $\pm$ 0.07 mJ/mol K respectively. 3This material is based upon work supported by the NSF (Grant Nos. DMR-0552458 (REU-Site) and DMR-0504799) and CAPES (Grant No. 0466/05-0).

K1.00217 Investigating the Diffusive Behavior of HPC with DLS and FPR: A Comparative Analysis of Experimental Method. RYAN MCDONOUGH, Cleveland State University, PAUL RUSSO, Louisiana State University, KIRIL STRELETZKY, Cleveland State University — The study of HPC (Hydroxy-propyl-cellulose) chains in aqueous solution through the experimental techniques of FPR (Fluorescence Photo-bleaching Recovery) and DLS (Dynamic Light Scattering) has shown empirical inconsistencies in observed polymer dynamics. The approach to analyzing the inconsistencies consisted of preparing fluorescein labeled and unlabeled HPC solutions at a range of concentrations from the same stock solution. Results from DLS have indicated the reliable presence of a slow mode of diffusion in both labeled and unlabeled samples. The slow mode appeared in FPR experiments, but not reproducibly. In addition, results from DLS on labeled and unlabeled HPC have found starting differences in line shape of correlation function indicating signal from an unknown mechanism. Future directions for this study include an investigation into the reasons behind the before mentioned inconsistencies and an analysis of HPC solutions with different fluorescent labels to further explore the nature of the slow diffusion mode if it is determined not to be an artifact from sample preparation, or an unknown aspect particular to DLS studies.

K1.00218 Investigation of the Oxidation Growth Kinetics of La$_{0.67}$Ba$_{0.33}$MnO$_3$ and LaMnO$_3$ Perovskite Films using Atomic Force Microscopy (AFM) lithography. MARC SCHNEIDER, MICHAEL EARLE, SANJAY ADHIKARI, MATT SNEIDER, KYLE HALL, RAJESwarI KOLAGANI, Towson University, DAVID SCHAEFER, Towson University — Manganese oxides doped with certain alkaline earth elements exhibit colossal magnetoresistance (CMR), which has great prospective applications in technological advancements. Our research is focused on the growth kinetics and electrical properties of LaMnO$_3$ and La$_{0.67}$Ba$_{0.33}$MnO$_3$. LaMnO$_3$, behaves as an anti-ferromagnetic and La$_{0.67}$Ba$_{0.33}$MnO$_3$ as a ferromagnetic material. The approach is based on a new way to generalize the so called “one way wave equation”. Our approach makes use some very simple,standard ideas from differential equations and the non-iterative solution of the Lippmann-Schwinger equation in quantum scattering. The importance of this new approach is that it corrects the usual approximation made in the one way wave equation so that the approach is equivalent to full solution of the two way acoustic scattering problem. However, because it is formulated so as to deal with coupled first order differential equations, it makes the problem appear to be one way. The initial conditions for the coupled first order differential equations need to satisfy the boundary conditions associated with waves that can travel two ways. The problem of evanescent waves is being treated using a projection operator technique patterned after an approach of H. Feshbach in nuclear physics. We are currently testing the method for several simple two dimensional acoustic models.

K1.00219 New Generalized Phase Shift Approach to Solve the Helomholtz Wave Equation. SAMEERA ABEBYKON, DONALD KOURI, University of Houston — A new method for solving the acoustic scattering wave equation in order to facilitate the exploration for production of oil and gas. The approach is based on a new way to generalize the so called “one way wave equation”. Our approach makes use some very simple,standard ideas from differential equations and the non-iterative solution of the Lippmann-Schwinger equation in quantum scattering. The importance of this new approach is that it corrects the usual approximation made in the one way wave equation so that the approach is equivalent to full solution of the two way acoustic scattering problem. However, because it is formulated so as to deal with coupled first order differential equations, it makes the problem appear to be one way. The initial conditions for the coupled first order differential equations need to satisfy the boundary conditions associated with waves that can travel two ways. The problem of evanescent waves is being treated using a projection operator technique patterned after an approach of H. Feshbach in nuclear physics. We are currently testing the method for several simple two dimensional acoustic models.

K1.00220 Characterization of 60 Hz environmental electromagnetic noise with a simple antenna. CHRISTOPHER HILL, RICHARD WILLIAMS, JOHN GAFFNEY, CHRISTOPHER SCHNEIDER, Southeastern Louisiana University, SATISH SHRESTHA, McNeese State University, SANICHIRO YOSHIDA, Southeastern Louisiana University, GIOVANNI SANTOSTASI, McNeese State University — The purpose of this project is to characterize environmental electromagnetic noise at 60Hz. We have constructed an antenna consisting of an LC circuit tuned around 60 Hz to detect the noise in the air, and made analyses in both the time and frequency domains. The data has shown considerable fluctuations in the peak frequency as well as the phase over any given period of time. Also, it has been found that the spectrum broadens depending on where the antenna is placed. We suspect that the broadening results from the superposition of seismic motion acting on the antenna to the electric signal. We are currently investigating if location and time of the day has any effect on the characteristics of the electromagnetic noise.
**K1.00221 Dynamics of a Planar Arm Model with Servo-regulated Viscoelastic Muscles in a Microgravity Environment**

JARED DURDEN\(^1\), Drury University Society of Physics Students — We constructed a mechanical arm model consisting of a rigid upper arm and forearm which simulates vertical planar arm motion with two degrees of freedom: shoulder rotation and elbow rotation. Computer controlled servo-motors effect rotation of the elbow and shoulder joints through tensions incited in elastic materials which represent muscles. We predicted and then observed vertical planar arm motion in the laboratory under normal Earth gravity conditions, and on NASAs Weightless Wonder in near zero gravity conditions. Because the arm only has two degrees of freedom we were able to simulate near zero gravity in the laboratory and predict the subsequent motion by operating it in the horizontal plane. We will discuss results of the actual observed motion in these three environments, and compare them to the motion predicted based on the equations of motion. We will also discuss how the project was developed physically, mathematically, and electronically.

\(^1\)Membership pending

**K1.00222 Why Not Solar Power?**

REEJU POKHAREL, PETER SHELDON, Randolph College (founded as Randolph-Macon Woman’s College) — Most of the world generally depends on energy sources such as fossil fuels and nuclear power to meet our energy consumption needs. As we all know, the excessive use of these resources has large environmental impacts, including displacing habitats, pollution, global warming, and scarcity of resources. Solar power is a clean energy source that has the potential to fulfill our energy needs while balancing the natural state of our environment. So why do we not power our houses with solar energy? I will give a general overview of the working principles of commercially available solar power, and examine the issues relating to why we should use it and why we currently do not.

**K1.00223 Ice Nucleation Near the Surfactant-Water Interface**

CALEB CARLIN, WILL CANTRELL, Dept. of Physics, MichiganTech University, CAROLINE TAYLOR, Dept. of Chemistry, MichiganTech University — Ice nucleation is a fundamental component of the atmospheric mechanisms driving the formation of clouds. Atmospheric nucleation occurs with a variety of compounds and conditions; but understanding the behavior of water is key in all cases. We have used multiscale molecular simulations to study heterogeneous nucleation in clouds, probing the influence of long-chain alcohols on the freezing of water droplets. Ice nucleation occurs at a finite distance from the heterogeneous surface, due to the disruption of the hydrogen bond network in response to the surfactant-water interface. The penetration depth of the disturbance is found to be dependent upon the chain length and surface organization, as well as the acidity of the terminal alcohol group.

**K1.00224 An Extended Hydrophobic Surface Submerged in Water: The Formation of a Depletion Layer**

COREY SHEMEhya, ADELE POYNOR, Allegheny College Physics Department — Hydrophobic literally means water hating. When small amounts of water come in contact with a hydrophobic surface, the water will minimize its contact area by forming a drop. What will happen when bulk water comes in contact with an extended hydrophobic surface? We have employed the surface sensitive technique of surface plasmon resonance to probe for the existence of a depletion region (an ultra-thin low-density region) at this boundary. We also explore the interaction of water and a mixed hydrophobic and hydrophilic surface and its effect on the formation of a depletion layer.

**K1.00225 ABSTRACT WITHDRAWN**

**K1.00226 PHYSICS EDUCATION**

**K1.00227 Physics Education for Blind Students: The Teachers’ Perspective**

AMAURI FERREIRA, Pontifícia Universidade Católica de Minas Gerais — We discuss the challenge high school teachers face when teaching physics to the blind. Using the oral history method, we interview physics teachers who have dealt with the inclusion of blind students in regular classrooms. Based on our study, we find that the performance of these students varies, depending on the studied subject. The narrative makes clear the teachers’ lack of preparation to deal with inclusion, and their search for alternative methods to improve blind students’ learning.

**K1.00228 Impact of Inquiry-Based Learning on Attitudes and Science Content Knowledge of Elementary School Teachers and Students\(^1\)**

PETER SHELDON, PEGGY SCHIMMOELLER, Randolph College (founded as Randolph-Macon Woman’s College) — We report on a research project studying the influence of hands-on and inquiry-based learning in K-8 classrooms. We designed learning experiences for teachers that included significant hands-on and inquiry-based lessons, and designed instruments to test attitudes and content knowledge. The lessons are meant to address topics of state and national learning standards. Teachers were invited to take part in a pilot program in the summer of 2006, and we hope to continue the project over the next few years. We will report on the activities developed, the attitudes toward and achievement in science, and any changes that were seen after learning science through active learning. Resources can be found on the project website, http://trst.randolphcollege.edu.

\(^1\)Partially supported by a Teacher Quality Enhancement Grant from the Virginia Department of Education

**K1.00229 Prospective Nanoscience Lessons for High School Classroom Activities**

JAETAE SEO, JAN MANQANA, COURTNEY DULA, OLIVIA KERWIN, JASMINE AUSTIN, THAMER KHASAWNEH, JENNIFER DO, LUIS GOITY, SEONGMIN MA, QIANGUANG YANG, BAGHER TABIBI, Hampton University, HAMPTON UNIVERSITY COLLABORATION, NORTHWESTERN UNIVERSITY COLLABORATION, PURDUE UNIVERSITY COLLABORATION — Workshops for learning and teaching in nanoscale science in the Hampton Roads area in Virginia have been provided for high school science teachers of 7-12th grade. Main objectives of the workshops are to enhance teachers’ awareness of the connections between nanoscience and the traditional sciences, and provide a collection of suitable classroom activities in nanoscience. Prospective nanoscience lessons for high school classroom activities have been introduced in summer 2007 and 08. The selected classroom lessons are surface area and volume, nanolight, solar cells, nanocard, allotropes of carbon, biosensors, DNA origami, ferrofluids, intermolecular forces, quantum dots, scanning probe microscopy, and space elevator. This work at Hampton University was supported by ARO (W911NF-07-1-0608) and NSF (HRD-0734635, HRD-0630372, and ESI-0426328/002).

**K1.00230 Modular Approach of Nanophysics for Undergraduate Science and Engineering Curriculum Development**

JAETAE SEO, EDMUND NDIP, JALE AKYURTULU, ATES AKYURTULU, Hampton University, HAMPTON UNIVERSITY COLLABORATION — Advances in nanoscience and nanotechnology are closely related with understanding nanoscale materials and their functionalization, which are still in their infancy. Further attention in the education of human-engineered nanoscale materials is needed before the beauty of nanoscience and nanotechnology becomes the reality of our modern life. The current urgent demand or existing challenge in nanoscience and nanotechnology is to educate, train, and prepare a new generation of skilled workers in nanoscience and nanotechnology. A modular approach of nanophysics for undergraduate curriculum development is introduced for educating students in multidisciplinary areas of science and engineering. The nanophysics educational modules are electronic dynamics and optical properties of semiconductor nanocrystals and nanomaterials. This work was supported by Army Research Office (W911NF-07-1-0608) and National Science Foundation (HRD-0734635, HRD-0630372, ESI-0426328/002, and EEC-0532472).
K1.00231 Quantum Mechanics Laboratories using Correlated Photons.\textsuperscript{1} , ENRIQUE GALVEZ, Colgate University — Progress in laboratory techniques with correlated photons has allowed the implementation of table-top experiments for teaching undergraduate quantum mechanics. The experiments that we have developed \textsuperscript{1} complement an undergraduate course on quantum mechanics. They use light at the quantum level to illustrate both fundamental and operational aspects of quantum mechanics. Laboratory experiments on interference of light with heralded photons, or with two correlated photons, going through an interferometer are vivid exercises on state superposition, state projection, and base rotation. Other experiments with entangled pairs address more fundamental aspects of quantum mechanics, including nonlocal correlations and violations of Bell Inequalities. \textsuperscript{[1]} E.J. Galvez et al., Am. J. Phys. 73, 127 (2005).

\textsuperscript{1} Funded by NSF grant DUE-0442882

K1.00232 Making the Nanoworld Accessible: Nanoscience Education Using Scanning Probe Methods\textsuperscript{1} , DANIEL KNORR, JASON KILLGORE, TOMOKO GRAY, DAVID GINGER, JOSEPH WEI, YEECHI CHEN, MEHMET SARIKAYA, HANSON FONG, TOM GRIFFITH, RENE OVERNEY — A partnership between researchers and educators at the University of Washington, North Seattle Community College and two companies, Nanosurf, AG and nanoScience Instruments has been forged to develop a nationally replicable model of a sustainable and up-to-date undergraduate teaching laboratory of scanning probe microscopy (SPM) methods applied to nanoscience and nanotechnology. Within this partnership a new paradigm of operating and maintaining a SPM laboratory has been developed that provides a truly hands-on experience in a classroom laboratory setting with a small student to instrument ratio involving a variety of SPM techniques and topics. To date, we have run a first successful undergraduate laboratory workshop, where students were able to have extensive hands-on experience on five SPM modes of operation including: electrostatic force microscopy involving photovoltaic polymeric materials, tunneling microscopy and the determination of the workfunction, and nanolithography using the dip-pen method.
http://depts.washington.edu/ nanolab/NUE\_UNIQUE/NUE\_UNIQUE.htm

\textsuperscript{1}This work is supported by the NSF under Grant No. 0634088.

K1.00233 Utilization of recycled neutron source to teach prompt gamma analysis activation-PGNA , CAMILO DELGADO-CORREAL, HECTOR MUNERA, university Nacional de Colombia — Neutron activation analysis based on prompt gamma ray emission has significantly developed during the past twenty years. The technique is particularly suited for the identification of low atomic number elements, as nitrogen that is a main component of drugs and explosives. Identification of these substances is important in the context of humanitarian demining, and in the control of illicit traffic of drugs and explosives. As a good example of recycling of radioactive sources, a $^{241}$Am-Be neutron source emitting $10^{7}$neutron/s, that was not longer in use for other purposes at Ingeominas, was used to build a neutron irradiator that can be used to teach prompt gamma ray analysis, and other nuclear techniques. We irradiated individual samples, each about 4 gram, of three different elements: nitrogen in urea, silicon in milled rock, and cadmium in cadmium oxide. The prompt gamma rays emitted in the nuclear reactions $^{112}$Cd (neutron,gamma) $^{113}$Cd, $^{29}$Si (neutron,gamma) $^{29}$Si and $^{14}$N (neutron,gamma) $^{15}$N were identified using a well-type NaI (Tl) detector, connected to a multi-channel analyzer.

K1.00234 Teaching Physics for Agronomy Students: Contextualizing Laboratory Classes \textsuperscript{1} , ANA LUCÍA NOGUEIRA, Universidade Estadual de Montes Claros, ADRIANA DICKMAN, Pontifícia Universidade Católica de Minas Gerais — In this paper we discuss a method of teaching physics to agronomy majors. We use laboratory classes to apply basic physics concepts to common situations in agronomy. As an example, we report a project developed by the students involving the construction of a device, frequently used on farms, to transport water without burning fuel or using electricity. We believe that contextualizing helps to improve physics classes and increase students’ motivation.

K1.00235 Measurement and simulation of AlSb/InAs triple barrier resonant tunneling diodes. NanoJapan program summer 2007\textsuperscript{1} , JEFFREY RUSSOM, KRISTJAN STONE, GSIST, Hokkaido University, Japan; Dept.of Physics and Astronomy, Rice University, TAKAAKI KOGA, GSIST and CRIS (Sousei), Hokkaido University, Japan; CREST, JST — Recently, Koga et al. \textsuperscript{1} proposed to make a spin filter out of only non-magnetic semiconductors. This spin filter consists of a triple barrier resonant tunneling structure (TB-RTS), and the Rashba spin-orbit coupling effect is utilized for matching the spin-dependent resonance levels, which would result in a high spin filtering efficiency. To test this theoretical idea, we obtained TB-RTS samples with InAs layers as quantum wells and AlSb layers as barriers from Tohoku University and studied their I-V characteristics. To understand the physics of our experimental $I – V$ curves obtained at 300, 77, and 4.2K, we also performed theoretical simulations. The authors acknowledge the growth of TB-RTS by Dr. K. Ohtani of Tohoku University. \textsuperscript{[1]} T. Koga, J. Nitta, H. Takayanagi and S. Datta, Phys. Rev. Lett. 88, 126601 (2002).

\textsuperscript{1}Supported by the Nano Japan Program of NSF and the CEED Internship Program of Hokkaido University

K1.00236 HISTORY OF PHYSICS —

K1.00237 Tracing the Rich History of Physics Research at NIST/NBS Through the Pages of the Journal of Research of the National Institute of Standards and Technology. SUSAN MAKAR, BARBARA SILCOX, National Institute of Standards and Technology — What do Edward B. Rosa, William W. Cobleantz, Ugo Fano, Charlotte E. Moore, William D. Phillips and Eric Cornell have in common? All are premier NBS/NIST physicists who published important research in the Journal of Research of the National Institute of Standards and Technology and the Journal’s precursors. The Journal of Research is the flagship publication of the National Institute of Standards and Technology, formerly the National Bureau of Standards. The Journal has been published under various titles and in various forms since 1904. This poster examines a sampling of the rich body of physics literature published in the Journal of Research since the early 1900s, and analyzes the impact this literature has had on the physics and scientific communities. From Edward B. Rosa’s paper, “The Absolute Measurement of Inductance” published in 1905, to the Journal’s 1996 Special Issue on Bose-Einstein condensation, the Journal of Research has been the venue for papers of some of the most influential American physicists of the twentieth century.

K1.00238 The Increasingly Disordered History of Entropy , CESAR RODRIGUEZ-ROSARIO, The University of Texas at Austin — The interpretation of irreversibility had played a significant part of philosophical debates, but it was not until Carnot and his son established entropy as part of the empirical science of engines that the issue reached practical importance. It also had to wait for Maxwell, Boltzmann, Gibbs and the birth of statistical mechanics that the concept of entropy was given a stronger theoretical basis, although the approximation it was based on is still a source of disagreement. This talk will focus on the debate from its early “demonic” times, past Szilard and Einstein building a refrigerator, to the role of von Neumann and Shannon in connecting the idea to information theory, without forgetting about the quantum mechanical master equations, all the way into its current use in quantum information theory.
K1.00239 The stolen brain of Einstein, KAVAN MODI, The University of Texas at Austin — Pathologist Thomas Stoltz Harvey performed an autopsy on Einstein after his death in 1955. During the autopsy Harvey removed Einstein’s brain, took pictures of it and then cut it into several pieces. A lot of scientific attention has been devoted to Einstein’ brain, and it still comes up once in a while. We’ve all heard something or other about Einstein’s brain, as it has become somewhat of a folk lore. What is less known is that Harvey in actuality did not have the permission to remove the brain. Only later pieces. A lot of scientific attention has been devoted to Einstein' brain, and it still comes up once in a while. We've all heard something or other about Einstein's

K1.00240 GENERAL THEORY INCLUDING SIMULATIONS OF MATTER AT EXTREME CONDITIONS; COMPUTATIONAL NANOSCIENCE; AND COMPUTATIONAL METHODS: MULTISCALE MODELING

K1.00241 Calculating cold curves for Equation of State using different types of Density Functional Theory codes, ANN E. MATTSSON, KYLE R. COCHRANE, JOHN H. CARPENTER, MICHAEL P. DESJARLAIS, Sandia National Laboratories, Albuquerque NM 87185 — With fast computers and improved radiation-hydrodynamics simulation techniques, increasingly complex high energy-density physics systems are investigated by modeling and simulation efforts, putting unprecedented strain on the underlying Equation of State (EOS) modeling. EOS models that have been adequate in the past can fail in unexpected ways. With the aim of improving the EOS, models are often fitted to calculated data in parts of the parameter space where little or no experimental data is available. One example is the compression part of the cold curve. We show that care needs to be taken in using Density Functional Theory (DFT) codes. While being perfectly adequate for calculations in many parts of the parameter space, approximations inherent to pseudo-potential codes can limit their applicability for large compressions. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

K1.00242 A Hybrid Density Functional Study of Zigzag SiC Nanotubes, KAZI ALAM, ASOK RAY — Using ab initio hybrid density functional theory based calculations, we report here the electronic and geometric structure properties of three different types of single-walled zigzag silicon carbide nanotubes from (3,0) to (11,0). Our calculations show type 1 structures to be most stable, with the cohesive energies of the newly proposed type 3 nanotubes intermediate between type 1 and type 2. For all nanotubes, Si atoms moved outward after relaxation making two concentric cylinders of Si and C atoms. The HOMO-LUMO (“band”) gaps for type 1 and type 2 nanotubes show an oscillatory pattern as the tube diameter increases but for type 3, the gap decreases monotonically with increasing tube diameter. All the tubes studied here appear to have triplet ground states except for type 1 (3, 0). It is expected that these tubes with significant surface reconstructions, varieties of band gaps, and magnetic properties would have interesting and important applications in the field of band gap engineering and molecular electronics.

K1.00243 Resonance modulations by tunable multi-level inter-dot coupling in a parallel quantum dot interferometer, YONG JOE, CHUNGHEE ROH, ERIC HEDIN, Ball State University, ARKADY SATANIN, Russian Academy of Science — We investigate the characteristics of resonance through parallel-coupled double quantum dots in an Aharonov-Bohm interferometer. In this system, we calculate the quantum transmission for different combinations of two-level inter-dot coupling by employing an exactly solvable tight-binding formalism. First, for the case that only one level in each dot participates in transport, we present contour plots of the transmission as a function of the energy level in each dot for different strengths of inter-dot coupling and magnetic flux. As the inter-dot coupling increases, an anti-crossing of resonances for a fixed magnetic flux appears due to the coalescence of two dots into one. In addition, a doubling of the periodicity in the transmission and the swing of the Fano resonance are also observed to be modulated by the magnetic flux. Second, for the case that two-levels in each dot contribute to the transport, an extra Fano resonance in the transmission appears by tuning the inter-dot coupling between the even–odd parity states. On the other hand, the inter-dot coupling of the odd-odd parity states gives rise to a collapse of the Fano dip in the transmission resonance. Finally, we discuss the resonance effect on the interplay between the two-level inter-dot coupling and magnetic flux.

K1.00244 Ab-Initio Molecular Dynamics Study of the Structural Stability of fcc-Carbon on Diamond, CHARLES CHIN-CANCHE, CESAR CAB, JORGE-ALEJANDRO TAPIA, Facultad de Ingenieria, Universidad Autonoma de Yucatan, GABRIEL MURRIETA, Facultad de Matematicas, Universidad Autonoma de Yucatan, ROMEO DE COSS, Departamento de Fisica Aplicada, Cineastav-Merida — The observation of a new carbon phase in thin films on diamond has been reported. High Resolution Electron Microscopy studies of the carbon thin films revealed a face-centered cubic (fcc) crystal structure with a lattice constant of 3.563 Å. It is interesting to note that this value is very close to that of carbon in the cubic diamond phase (3.567 Å), suggesting that the substrate is contributing to the stabilization of fcc-carbon. Thus, in the present work we have studied the structural stability of fcc-C on the surface (001) of diamond. We have used the Density Functional Theory and the Molecular Dynamics approach in the slab configuration. The calculations where performed with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have analyzed the changes in the atomic structure, density of states (LDOS), and the local orbital population. We found that the carbon layers in the fcc structure on diamond are unstable.

K1.00245 A coarse-grained model for simulations of graphite and carbon nanotubes, ALPER BULDUM, Department of Physics, The University of Akron, Akron, OH 44325, TOSHIIYUKI OHASHI, Honda Research Institute USA, Inc., Columbus, OH, 43212, LIMING DAI, Department of Chemical and Materials Engineering, University of Dayton — As multi-walled nanotubes in many experimental systems are quite large in diameter and in length and they consist billions of atoms, a new multi-scale modeling approach is necessary. This modeling approach can serve as a bridge between atomistic modeling and continuum modeling of multi-walled nanotubes. For graphite nanobeams and carbon nanotubes we present a new model which is based on the hexagonal symmetry of the graphite structure. This model is based on “N cell to one Cell” mapping of the graphite structure. N cells in the original atomic structure are equivalent to one cell in the hexagonal mesh model. The number N can be very large thus it is possible to model large multi-walled nanotubes and graphite nanobeams.
K.00246 Linking Quantum and Classical Descriptions: Hierarchical Development of Born-Oppenheimer-like Approximations. YING HU, Department of Physics and Astronomy, Vanderbilt University — The Born-Oppenheimer (BO) approximation is ubiquitous in quantum mechanical calculations of molecular wavefunctions. Here I report an extension of traditional BO approximation to a hierarchy of BO-like approximations which enables dynamic linking among distinct scales in complex crystals, from the quantum world to the macroscopic. At first, the usual BO approximation allows us to average out electrons to give descriptions of slow motion of nuclei. Then we describe an atom in crystals with two classes of independent variables corresponding to two distinct time scales: lattice deformation and relative atomic motion. We invoke a BO-like Ansatz as constraint to construct a ‘constrained distribution function’ so that phonons are averaged out from lattice deformation. To progress further, we use BO-like approximation to modify constraints so as to account for defects. The BO-like approximations is further extended from separating distinct time scales to different length scales. The ultimate hierarchy of BO-like approximations enables formulation of nonequilibrium multiscale statistical mechanics where electrons, phonons, defects and lattice deformation are dynamically coupled.

K.00247 Gas Adsorption Characterization of Rigid and Amorphous Polymers. GREGORY LARSEN, Penn State University, FLOR SIPERSTEIN, PETER BUDD, The University of Manchester, CORAY COLINA, Penn State University — Nanostructured materials have unusual mechanical, electrical and optical properties and are becoming increasingly important for energy storage. A variety of materials, such as zeolites, metal organic frameworks, covalent organic frameworks, activated carbons, and hypercrosslinked polymers, have recently been explored for energy storage. Polymers of Intrinsic Microporosity (PIMs) are macromolecules that form nanoporous materials (effective pore size <2 nm) that are rigid at a nanometer length scale due to the structure of the selected monomers, but can be flexible at a macroscopic scale and show swelling properties due to their polymeric nature. PIMs offer an interesting alternative to the materials mentioned above, as the functionality can be directly embedded in the material framework, allowing for intrinsic control in adsorptive properties by the PIM and flexibility in alternate adsorption applications such as CO2 sequestration. In this work, we present our recent efforts to study PIMs by MC simulations, and demonstrate the effects of box size and chain length on simulated measurements including pore size distribution and surface area.

K.00248 FLUIDS AND SOFT MATTER —

K.00249 Is the energy landscape of simple fluid a fractal?. GERARDO NAUMIS, Depto. de Física-Química, Instituto de Física, UNAM — The energy landscape of fluids is known to be very important close to a phase or glass transition. Real landscapes are fractal objects so one can ask if something similar happens with the structure of the phase space topology. Thus, a simple modification of the Monte-Carlo algorithm is proposed to explore the topography and the scaling of the energy landscape. We apply this idea to a simple hard-core fluid. The results for different packing fractions show a power law scaling of the landscape boundary, with a characteristic scale that separates the values of the scaling exponents. Finally, it is shown how the topology determines the freezing point of the system due to the increasing importance and complexity of the boundary.

K.00250 Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of liquid lead1. L.J. GALLEGOS, MANUEL ALEMANY, R.C. LONGO, Universidad de Santiago de Compostela, Spain, D.J. GONZALEZ, L.E. GONZALEZ, Universidad de Valladolid, Spain, MURILO L. TIAGO, Oak Ridge National Laboratory, JAMES R. CHELIKOWSKY, University of Texas at Austin — We present results for a comprehensive study of the static, dynamic and electronic properties of liquid Pb near melting by means of 216-particle ab initio molecular dynamics simulations based on a real-space implementation of pseudopotentials constructed within density-functional theory. The predicted results and available experimental data are in very good agreement, which confirms the accuracy of this technique to achieve a reliable description of the behavior of liquid metals, including their dynamic properties. Although some of the computed properties of liquid Pb are similar to those of simple liquid metals, others differ markedly. Our results show that an appropriate description of liquid Pb requires the inclusion of relativistic effects in the determination of the pseudopotentials of Pb.

1 Work supported by the Spanish Ministry of Education and Science (Program Ramon y Cajal and Projects FIS2005-04239 and MAT2005-03415), by the NSF (Project DMR-0551195), by the DOD (Projects DE-FG02-06ER46286 and DE-FG02-06ER15760), and by CEGSA.

K.00251 Critical fluctuations and phase separation in pure fluid1, ANA OPRISAN, SORINEL OPRISAN, GREG SMITH, College of Charleston, JOHN HEGSETH, University of New Orleans — A series of experiments were performed in microgravity in order to study fluctuations and phase separation in pure fluids. These experiments were performed using Alice 2 apparatus containing an optical cell filled with sulfur hexafluoride (SF6) near critical point. Fluctuations of the intensity of the transmitted light through a cell containing the fluid under investigation appear as domains of different intensities. Critical fluctuation images are very sensitive to optical noise from the experimental system. Two different methods used in image processing were tested and the results in order to find the optimal filtering method. First method is based on an n-point filter to eliminate optical noise from images obtained in microgravity. The second method is based on wavelets threshold to eliminate optical noise. We also estimated the fractal dimension of the images. For the critical fluctuations the characteristic length of the fluctuations and the fractal structure factor were estimated. The temporal evolutions of concentration fluctuations were also analyzed and the correlation time was determined. The Schlieren technique was also used to image ultrasound beam incident on a corrugated water-brass interface and showed a backward displacement of the reflected beam at an angle of 22.5°, confirming the observations of Breazeale and Torbett [Appl. Phys. Lett. 29, 456 (1976)]. However, a new theory hypothesizes that this beam displacement results from excitation of a new type of leaky surface wave.

1 NASA-OBPs grant NAG3-2447, RGD grant -College of Charleston

K.00252 Imaging density fluctuations in liquids using Schlieren photographic technique, ANA OPRISAN, SORINEL OPRISAN, ALEM ABRAHA TEKLU, College of Charleston — Schlieren imaging method was used to visualize variations in the index of refraction or density of transparent liquid media. In one set of experiments, a colloidal suspension of silica and water was placed in a sample cell of 20 mm height. Schlieren method was used to visualize non equilibrium fluctuations caused by a concentration gradient. Using image processing techniques, the characteristic length of the fluctuations and the static structure factor were estimated. The temporal evolutions of concentration fluctuations were also analyzed and the correlation time was determined. The Schlieren technique was also used to image ultrasound beam incident on a corrugated water-brass interface and showed a backward displacement of the reflected beam at an angle of 22.5°, confirming the observations of Breazeale and Torbett [Appl. Phys. Lett. 29, 456 (1976)]. However, a new theory hypothesizes that this beam displacement results from excitation of a new type of leaky surface wave.

K.00253 Deep supercooling and relaxation processes in confined liquid crystals. FOAUD ALIEV, EDWIN ARROYO, SARMISTHA BASU, MANUELE RIVERA, University of Puerto Rico — Broadband dielectric and photon correlation spectroscopies has been applied for investigations of the dynamic behavior of liquid crystals (LCs) confined in porous matrices with random pores. We observed deep supercooling of LC in random pores. The relaxation times of the process due to the molecular reorientations in deeply supercooled state are slower than at the temperatures corresponding to nematic phase by a 5-6 orders of magnitude. This slowing down is accompanied by anomalous broadening of the dielectric spectra. The relaxation processes due to reorientation of molecules (of liquid crystals confined in narrow random pores) around their short axis is glass-like and the temperature dependence of relaxation times obeys Vogel-Fulcher law. Dynamics of director orientational fluctuations was also strongly affected by random confinement and these fluctuations were not frozen at temperatures much below bulk crystallization temperature. The small pore size (surface effects) and random pore structure (geometrical disorder) stimulate partial disorder (at least at long scales) and prevent crystallization. Therefore LC supercooled in small random pores has properties typical for glass forming liquids.
K1.00254 A study of electric field response by liquid crystal molecular dynamics algorithm. JONES TSZ-KAI WAN, Department of Physics, The Chinese University of Hong Kong — The response to an electric field of a liquid crystal cell is studied by the newly developed liquid crystal molecular dynamics (LCMD) algorithm. In contrast to the conventional conjugate gradient (CG) approach, which can only simulate the initial and final configurations of a LC cell under an applied electric field, the LCMD scheme can simulate intermediate configuration of the LC molecules. In addition, the electric field distribution within the LC cell at each time step is calculated directly. In this way, three cases will be presented: (i) LC molecules with spatial variation of polar angle, (ii) LC molecules with spatial variation of azimuthal angle and (iii) LC cells with nano-scale patterned substrates. The optical properties of the intermediate LC cell will also be presented.

K1.00255 Electro-optic properties of liquid crystal carbon nanotube composites. GEORGI GEORGIEV, Assumption College. YANIEL CARRERA, Tufts University. MARK CROWN, CHRISTOPHER ROCHELEAU, ZARNAB IFIHKAR, Assumption College. PEGGY CEBE, Tufts University. TUFTS UNIVERSITY COLLABORATION, ASSUMPTION COLLEGE COLLABORATION — We study the effects of carbon nanotubes on different properties of different liquid crystals: the elastic constant, Freedericksz transition, topological defect formation, interaction with external fields (i.e. electric). During our previous studies on the altitudinal angle of carbon nanotube doped liquid crystal electro-optic cells, we have measured a large shift of the transition voltage during Freedericksz transition. We are continuing our exploration on the physical properties of the liquid crystal nanocomposites. One of the most interesting questions is how different types of carbon nanotubes, conductive and semi-conductive affect the electrical properties of the liquid crystals. Our main tool is two dimensional microscopic transmission ellipsometry which provides information about the 3D orientation of the liquid crystalline entities.

K1.00256 Environmental Mode SEM Studies of Liquid Crystal Droplets. KASHMAI RAI, ADAM FOTEC-CHIO, Drexel University — An in-depth understanding of the liquid crystal nanometer scale structure of the holographic polymer dispersed liquid crystals (HPDLCs) is essential to optimally improve its diffraction efficiency. In this work the liquid crystal (LC) droplets are imaged for the first time in HPDLCs without LC removal using environmental mode SEM (ESEM). The field controllable HPDLCs have periodic layers of LC droplets and polymer matrix. Their applications include photonic crystals, optical pressure sensors, reconfigurable mirrors, wavelength filters and displays. Hi-vac mode SEM is a well-known technique used for high-resolution structural analysis of HPDLCs where the LC is removed prior to imaging. This results in the contractions and sometimes collapsing of grating structure. ESEM imaging aid in the study the LC microscopic structure without LC removal. A comparison of morphology features such as grating thickness, droplet structure is made between the images obtained by ESEM and hi-vac SEM.

K1.00257 Diffusion and micro-structure of dense liposome suspensions. YAN YU, Dept of Materials Science & Engineering, University of Illinois at Urbana-Champaign, STEPHEN M. ANTHONY, Dept of Chemistry, University of Illinois at Urbana-Champaign, SUNG CHUL BAE, STEVE GRANICK, Dept of Materials Science & Engineering, University of Illinois at Urbana-Champaign — Phospholipid vesicles can be stabilized against fusion, up to volume fraction around 80%, which is accomplished by studding the outer leaflet with charged nm-sized particles. The diffusion of such soft, flexible and hollow objects is revealed by single-particle tracking. Image analysis of time trajectories, obtained using epifluorescence imaging, was performed at sub-pixel resolution. This poster will reveal aspects of curiously heterogeneous dynamics and also quantification of microstructure in this system. Taken together, this system of charged, polydisperse, flexible objects displays rich dynamics that contrasts acutely with known behavior for hard-sphere dense particle systems.

K1.00258 Emulsions stabilized by Janus amphiphilic colloidal particles. SHAN JIANG, MITCH SCHULTZ, QIAN CHEN, JEFFREY MOORE, STEVE GRANICK, University of Illinois at Urbana-Champaign — Emulsions stabilized by amphiphilic colloidal particles were investigated by both theoretical calculation and experiments. The concept of Janus balance is defined as the dimensionless ratio of work to transfer an amphiphilic colloidal particle (a ‘Janus particle’) from the oil-water interface into the oil phase, normalized by the work needed to move it into the water phase. The calculation shows that the emulsion will be most stable when the Janus balance is unity. Experimentally, large quantities of Janus particles with different Janus balance were synthesized. The emulsion type and emulsion stability were investigated by using these particles to stabilize oil-water emulsions. It is found that Janus particles can stabilize emulsions for extended times. Finally, the emulsion type will be shown to depend on the geometry (Janus balance) of the Janus particles.

K1.00259 Flow-induced Shear of Colloidal Gels. TIFFANY SOO, GARY HUNTER, ERIC R. WEEKS, Emory University — We study colloidal gels as they break apart under shear. To make our colloidal gels, we add polyisocyanate polymer to PMMA colloids, inducing the depletion force. We then pump these colloidal gels through a capillary tube, and the resulting parabolic flow profile in the tube causes the gel to shear and break. We visualize this using confocal microscopy. We present two-dimensional and three-dimensional data from this experiment that has been analyzed through tracking individual particles and the movement of aggregates. We study the breaking points of the gel and characterize the structure of these points as a function of flow rate, volume fraction, and polymer concentration.

K1.00260 Effect of the polydispersion in the crystallization and micro-structure of the high charged colloids. EFRAIN URRUTIA-BÁÑUELOS, Universidad de Sonora, HELIM ARANDA-ESPINOZA, Department of Bioengineering University of Maryland, MARTIN CHASVEZ-PAEZ, Instituto de Fisica de la Universidad Autonoma de S.L.P. — In this work we investigate the effect of the polydispersion in the crystallization and micro-structure of the high charged colloids particles with tow and three different types and different concentrations of that types. This results were obtained by computer simulation, the particles interaction was modeled by a screened Coulomb potential. We used 4000 particles in our simulation cell to let them evolve from an initial random configuration, periodic boundary conditions was imposed to simulate the bulk. The temporal evolutions of the configuration show long-range self-ordering and a crystalline transition, the crystalline nucleation depend of the concentrations of different kinds as well as of types of particle. The common neighbor analysis (CNA) exhibits the competition of two micro-structures, icosahedral and bcc, in the equilibrium bcc crystalline order is dominant with relative abundance over the other micro-structures. 1. - U. Gasser, Eric R. Weeks et al, Science, 292 (250), 2001. 2. - Stefan Auer, Daan Frenkel, Letter of Nature, 400 (1020), 2001. 3. - J.P. Hoogenboom, et al, Phys. Rev. Letters, 89 (256104), 2002. 4. - M. Chávez-Pérez, E. Urrutia-Bañuelos and M. Medina –Noyola, Phys. Rev. E, 58 (681),1998 5. - Andrew S. Clarke and Hannes Jónsson, Phys. Rev. E, 47 (3975), 1993.

K1.00261 Using DLS Spectroscopy and Optical Probe Diffusion to examine structure of Brij Micelles. KAREN WILLIAM, MIKE LEKAN, KIRIL STRELETZKY, Cleveland State University — We studied properties of Brij-35 surfactant micelles in solution using Dynamic Light Scattering (DLS) Spectroscopy and Optical Probe Diffusion method. Aqueous solutions of Brij-35 with concentrations ranging from 2 to 100g/L were prepared, both with and without polylysene latex probes of diameters 24, 50, 186, 282 and 792nm. Solutions were studied at four temperatures of 10, 25, 40 and 70°C with DLS to obtain micelle and probe diffusion coefficients (D_m, D_p). Using both diffusion coefficients we deduced micelle radius (a_m), micelle water content (δ), and number of surfactant molecules per micelle (N) using two different models. First, hard sphere model of micelles/probe interaction was used to analyze the data by two methods, after a_m was obtained from intercept of D_m(c). The first method uses the slope of D_m(c) and size of probes to determine N and δ. The second method uses the linear least-squares fit of D_m(c) for different probe sizes to determine N and δ. Both methods reveal that with increase in solution temperature a_m increases by 10%, N increases and δ decreases by a factor of 2. The second model treats micelles as core-shell particles with corona radius (a_c). This model used two different approaches based on linear least-squares fits of D_m(c) and D_p(c). We found a_c to be 4.45nm and a_m to be 1nm without relying on Stokes-Einstein equation. Results for N and δ were also consistent.
K1.00262 von Karman Vortex Streets Generated by Different Shaped Rods, ILDOO KIM, University of Pittsburgh, RORY CERBURSE, Purdue University, XIAO-LUN WU, University of Pittsburgh — von Karman vortex street is a pattern of vortices behind a bluff body in a uniform stream. Strouhal number St, a non-dimensional frequency of vortex shedding, depends on Reynolds number Re, however the precise relationship is not known although there were several proposals. To test these proposals and to investigate the nature of vortex shedding, we have generated von Karman vortex streets in two-dimensional soap film using conic bodies with different cross-sectional geometric shapes and orientations. We found that the structure-based St-Re relationship, St=1/(A+B/Re), is in good agreement with our experimental data using different shapes and orientations. Two coefficients A and B are functions of geometries and orientations of bluff bodies. Also, we found under certain conditions, two adjacent vortices merge into a big vortex downstream.

K1.00263 Electrostatic gyrokinetic turbulence, GABRIEL PLUNK, UCLA — A kinetic description of turbulence becomes necessary in cases where particle collisions are not strong enough to maintain a local Maxwellian velocity distribution over relevant dynamical timescales. This is often the case with plasmas. This type of turbulence can exhibit structure formation in phase space having, in general, double the dimensionality. We study a simple limit of the gyrokinetic equation where there are two spatial dimensions and one velocity dimension. Symmetries are exploited to find scaling laws using standard arguments from neutral fluid turbulence. A discussion of closure is presented with an emphasis on the relationship to Navier-Stokes turbulence and the kinetic extension of the Navier-Stokes equation, the Boltzmann equation.

K1.00264 Microfluidic cell electroporation using a mechanical valve, CHANG LU, JUN WANG, M. JANE STINE, Purdue University, West Lafayette, IN, BIOLOGICAL ENGINEERING TEAM — A microfluidic electroporation technique is demonstrated based on the operation of an elastomeric valve in a polydimethylsiloxane (PDMS) fabricated microchip and a common dc power supply. The pulse needed for permeabilization of the cell membrane is generated by temporarily interrupting the circuit using the valve. The electroperoxemabilization of suspended and adherent Chinese hamster ovary cells with green DNA dye SYTOX is demonstrated. The technique eliminates the cost and complexity associated with a pulse generator and microfabricated electrodes that are often involved in microscale electroporation devices. It also offers the potential of integrating electroporation as a unit operation in large-scale microfluidic systems with the increasing application of elastomeric valves in these systems.

K1.00265 Ionic currents through individual carbon nanotubes, CHRISTINE MEYER, MARC ZUDDAM, VISHAL MERANI, JEROEN DE GREBBER, CEES DEKKER, Kavli institute of nanoscience, Delft University of Technology, The Netherlands — The miniaturization from microfluidic to nanofluidic channels is a growing field of research. Many new effects are predicted and observed in nanochannels owing to the increased influence of surface interactions. One of the most intriguing features is the theoretical prediction by Hummer et al (2001) of an enhanced flow of aqueous solutions through hydrophobic carbon nanotubes. Experimental work has so far been done on membranes of carbon nanotubes (Hinds et al., Holt et al.). To the best of our knowledge, the experimental investigation of fluid flow through an individual single-wall carbon nanotube has not been conducted. We have developed a fabrication scheme that allows us to do measurements on such individual tubes. It is based on the use of a sacrificial layer etching process to fabricate connections to the nanotube. First measurements reveal that the ionic current through an individual 2 micron long single-wall nanotube is slightly smaller than expected from geometrical considerations. We hope to be able to present more extensive experimental data, e.g. on the variations between individual carbon nanotubes having the same nominal parameters.

K1.00266 Toward a Carbon Nanotube-Based Capillary Rheometer, NEAL SCRUGGS, JOSEPH ROBERTSON, JOHN KASIANOWICZ, KALMAN MIGLER, National Institute of Standards and Technology — Nanofluidic devices featuring multi-walled carbon nanotubes (MWNTs) as fluid channels are fabricated for the purpose of measuring the flow of individual, submicron objects (e.g. polymers, nanoparticles) in solution. (Sun, Crooks J. Am. Chem. Soc. 122, 12340, 2000) The MWNTs serve as conduits between two electrolyte reservoirs and the passage of an analyte through (MWNTs) as fluid channels are fabricated for the purpose of measuring the flow of individual, submicron objects (e.g. polymers, nanoparticles) in solution.

K1.00267 Sequential random packings1, PEDRO LIND, Institute for Computational Physics, Universitaet Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany — We introduce sequential random procedures to pack polydisperse particles, for both cases of spherical and ellipsoidal shape. In the case of spheres, we generalize the recent research of random space-filling bearings to a more realistic situation, where the spacing offset varies randomly during the space-filling procedure, and show that it reproduces well the size-distributions observed in recent studies of real fault gouges. In particular, we show that the fractal dimensions of random polydisperse bearings sweep predominantly the low range of values in the spectrum of fractal dimensions observed along real faults, which strengthen the evidence that polydisperse bearings may explain the occurrence of seismic gaps in nature. For ellipsoids we discuss the main difficulties in packing polydisperse ellipsoids sequentially and propose a procedure to overcome them, based in variational methods.

1 This work was supported by Deutsche Forschungsgemeinschaft, under the project LI 1599/1-1.

K1.00268 The stress dip under a granular semi-pile., TOM MULLIN, University of Manchester, IKER ZURIGUEL, University of Navarro — The origin of stress dip under the apex of a sandpile has stimulated significant debate within the scientific community. On the other hand, it is argued that a semi-pile built against a vertical wall is of more practical interest since it serves as a model of dams, dykes and embankments. Numerical results suggest that stress dip will not be a dip in this case. Here we show clear experimental evidence that the presence of the wall enhances the dip under the pile significantly. Moreover, our investigation provides insight into the influence of the wall on the force chains which appear to be a key element in the formation of the dip.

1 Support from EPSRC

K1.00269 Discrete Element Modeling of Close Box Oscillation with Granular Particles: Force Laws and Energy Dissipation, XIANG-MING BAI, LEON KEER, JANE WANG, RANDALL SNURR, Northwestern University — Partially filled cavity particle dampers are widely used in aerospace applications. In comparison to the conventional viscous fluid based damping, the temperature-independent performance and design simplicity of particle dampers make them more attractive when the temperature varies significantly. Recently, the discrete element method (DEM) has been widely used to simulate the particle damper consisting of a cavity box. In order to truly represent the real damping system, the use of accurate force laws in the DEM simulation is critical. In this work, we use different force models in DEM simulation to investigate the damping behavior of a close oscillating box filled with glass and steel particles. The force models used in this work include linear, Hertz, inelastic, plastic, history-dependent, and history-independent models. We note that the damping is very sensitive to the shear force models, but insensitive to the normal force models. The underlying mechanism has been investigated. In order to investigate the optimum filled fraction of particles and help us design the dampers, various configurations of different filled fractions are simulated. The energy dissipation through collision and friction is also investigated in this damping device.
K1.00270 The Transition of Two-Dimensional Hard Spheres from Liquid to Solid Regimes Under Gravity Using a Global Equation of State. ALISON KOSER, PAUL QUINN, Kutztown University of Pennsylvania — In a previous paper, Hong started with the Enskog equation for hard spheres of mass $m$ and diameter $d$ under gravity, and derived an exact equation for an equilibrium density profile at a specific temperature $T$. [Physica A, 271, 192 (1999)] This leads to a transition between the liquid and the solid regime that is temperature dependent. The size of the solid regime can be predicted using the temperature of the system obtained from the density profile. In a previous paper, Luding derives a new global equation of state for hard spheres in two-dimensions under gravity. [Phys. Rev. E, 163(2001)] Using this equation, we obtain a more exact equation for an equilibrium density profile at a temperature $T$ in two-dimensions. We use this equation with MD simulated data to obtain relationships of the number of solid layers, the center of mass, and the fluctuations of the center of mass as a function of $T$.

K1.00271 ABSTRACT WITHDRAWN –

K1.00272 Solitary granular avalanches: stability, fingering and theoretical modeling. FLORENT MALLOGGI, BRUNO ANDREOTTI, ERIC CLEMENT, ESPCI - University of Paris 6, Paris, France, IGOR ARONSON, Argonne National Laboratory, USA, LEV TSIMRING, INS-University of San Diego, USA — Avalanching processes do not only occur in the air as we know of snow avalanches, mud flows and landslides. Such processes can be naturally found and studied also on a microscopic scale, such as they take place from turbidity currents to thick sediment waves. In this study, we report results on laboratory scale avalanche experiments taking place both in the air and under-water. In both cases a family of stable solitary erosion/deposition waves is observed [1]. At higher inclination angles, we show the existence of a long wavelength transverse instability followed by a coarsening and the onset of a fingering pattern. While the experiments strongly differ by the spatial and time scales, the agreement between the stability diagrams, the wavelengths selection and the avalanche morphology suggest a common erosion/deposition scenario. We also use these erosion/deposition waves to investigate the dynamics of granular flow and jamming in the frame work of the Partial Fluidization Theory (PFT) proposed by Aronson et al. to describe the dynamics of granular matter near jamming [2]. [1] F. Malloggi et al. Europhysics Letters, 2006, Erosion waves: Transverse instabilities and fingering, 75, 825-831 [2] I. S. Aranson et al. Transverse instability of avalanches in granular flows down an incline. Physical Review E, 2006, 73, 050302; I.S.Aronson et al., Non rheological properties of granular flows: exploring the near jamming limit, preprint (2007).

K1.00273 Examination of the Angle of Repose in a Vertically Vibrated Container of Granular Materials. CARL FAUST, PAUL QUINN, Kutztown University of Pennsylvania — Experiments are conducted using various granular materials subject to a vertical vibration. The angle of repose is studied while varying certain parameters of the system, such as vibration amplitude, vibration frequency, initial height, grain size, container size, and container shape. Empirical relationships are found for the angle of repose as a function of each of these variables. Precession of the angle of repose is also examined, particularly as a function of grain size.

K1.00274 Relative Permeabilities: a pore-level model study of the capillary number dependence. MARTIN FERER, GARY MASON, Physics, West Virginia University, GRANT BROMHAL, DUANE SMITH, U.S.; D. O. E.; National Energy Technology Laboratory — Relative permeabilities are widely used by the petroleum industry in reservoir simulations of recovery strategies. In recent years, pore-level modeling has been used to determine relative permeabilities at zero capillary number for a variety of more and more realistic model porous media. Unfortunately, these studies cannot address the issue of the observed capillary number dependence of the relative permeabilities. Several years ago, we presented a method for determining the relative permeabilities from pore-level modeling at general capillary number. We have used this method to determine the relative permeabilities at several capillary numbers and stable viscosity ratios. In addition, we have determined these relative permeabilities using one of the standard dynamic methods for determining relative permeabilities from core flood experiments. Our results from the two methods are compared with each other and with experimental results.

K1.00275 Analysis of Drop Oscillations Excited by an Electrical Point Force in AC EWOD. JUNG MIN OH, SUNG HEE KO, KWAN HYOUNG KANG, Dept. of Mech. Eng., POSTECH, San 31, Hyoja-dong, Pohang, South Korea — Recently, a few researchers have reported the oscillation of a sessile drop in AC EWOD (electrowetting on dielectrics), and some of its consequences. The drop oscillation problem in AC EWOD is associated with various applications based on electrowetting such as LOC (lab-on-a-chip), liquid lens, and electronic display. However, no theoretical analysis of the problem has been attempted yet. In the present paper, we propose a theoretical model to analyze the oscillation by applying the conventional method to analyze the drop oscillation. The domain perturbation method is used to derive the shape mode equations under the assumptions of weak viscous flow and small deformation. The Maxwell stress is exerted on the three-phase contact line of the droplet like a point force. The force is regarded as a delta function, and is decomposed into the driving forces of each shape mode. The theoretical results on the shape and the frequency responses are compared with experiments, which shows a qualitative agreement.

K1.00276 Apparent Slip at Hydrophilic Surface: Fluorescence Resonance Energy Transfer. CARL FAUST, PAUL QUINN, Kutztown University of Pennsylvania — Experiments are conducted using various granular materials subject to a vertical vibration. The angle of repose is studied while varying certain parameters of the system, such as vibration amplitude, vibration frequency, initial height, grain size, container size, and container shape. Empirical relationships are found for the angle of repose as a function of each of these variables. Precession of the angle of repose is also examined, particularly as a function of grain size.

K1.00277 Effect of surfactants on the film thickness in the drag-out coating problem. PRABIR DARIPA, Texas A&M University — In this paper, we give a simple proof of the thickening effect of surfactant on the thin film deposited when a flat plate is withdrawn from a liquid bath. This problem without the effect of surfactant was first considered in the seminal paper of Landau and Levich (1942). Our proof here is based on an asymptotic analysis of the lubrication model for the Navier-Stokes equations. Our result is consistent with the results obtained numerically and experimentally on similar problems by other investigators. We will discuss our result against the backdrop of these known numerical and experimental results. This result has been obtained in collaboration with Gulu Pasa.

K1.00278 Self-consistent fluid-plasma simulation in small spaces. MANISH JUGROOT, Royal Military College of Canada — There is a great interest in understanding fluids and plasmas in small spaces as the complexity of micro technology systems increases. A self-consistent model of charged and fluid particle dynamics is applied to atmospheric small space (200 μm) discharges in helium. Hydrodynamic transport equations of the self-consistent model are described with an emphasis on the different terms involved in the close coupling among the fluid species, charged species and the electric field. The discharges are studied from an initial cloud till the stages of charged particle over-amplification in small spaces where transients are particularly important. Gas heating, neutral depletion and electric field reversals are observed, highlighting the close interaction between fluid and charged species – both effects therefore characterize and govern the evolution of the small space discharge.
K1.00279 Relaxation Dynamics in Glass-Forming Hydrogen-Bonded Liquids, H.G.E. HENTSCHEL, Emory University, ITAMAR PROCACCIA, Weizmann Institute of Science — We will address the relaxation dynamics in hydrogen-bonded super-cooled liquids near (but above) the glass transition, measured via Broad-Band Dielectric Spectroscopy (BDS). We propose a theory based on decomposing the relaxation of the macroscopic dipole moment into contributions from hydrogen bonded clusters of molecules. We discuss the statistical mechanics of the super-cooled liquid and with a theoretical estimate of the relaxation time of each cluster we provide predictions for the real and imaginary part of the frequency dependent dielectric response. Using glycerol as a particular example we demonstrate quantitative correspondence between theory and experiments. The theory also demonstrates that the ε peak and the “excess wing” stem from the same physics in this material.

K1.00280 Breakdown of effective temperature agreement near jamming, ADAM ABATE, DOUG DURIAN, University of Pennsylvania — The jamming concept may unify a wide class of disparate phenomena. Central to this is the behavior of effective temperatures as a system falls out of equilibrium. We present experimental measurements of effective temperatures in a granular system as it is gradually brought close to jamming. One effective temperature is based on the Einstein relation and defined in terms of the ratio of diffusion to mobility of a heavy test particle dragged through the system. The others are measures from local single-particle observables: the granular temperature is the average kinetic energy of the grains; the thermostometer temperature is the average total mechanical energy of a weighted oscillator placed in the system. In thermal equilibrium and, surprisingly, when this non-equilibrium granular system is driven far from jamming, these effective temperatures agree. As jamming is approached, the Einstein temperature, which depends on system wide relaxation, systematically deviates from the other local measurements of effective temperature. The amount of deviation depends on the system’s proximity to jamming and results in qualitative scaling differences of the relaxation timescales. These results suggest that global packing constraints play an important role in the breakdown of the thermal analogy as granular materials jam.

K1.00281 Crystal growth kinetics exhibit a fragility-dependent decoupling from viscosity, MARK EDGER, University of Wisconsin-Madison, PETER HARROWELL, University of Sydney, LIAN YU, University of Wisconsin-Madison — We establish the temperature dependence of the kinetic coefficient associated with crystal growth into the supercooled liquid for 7 organic and 8 inorganic materials. We show that the kinetic coefficient for crystal growth scales with the shear viscosity raised to an exponent that depends systematically on the fragility of the liquid; fragility quantifies the deviation away from an Arrhenius temperature dependence for the viscosity. For strong liquids, the exponent is -1. The greater the fragility, the larger the deviation from -1. We argue that this breakdown in scaling between the crystal growth kinetics and the viscosity is a manifestation of heterogeneous dynamics in supercooled liquids.

K1.00282 Dynamics in depletion gels studied with X-ray photon correlation spectroscopy, ANDREI FLUERASU, ABDELLATIF MOUSSAID, European Synchrotron Radiation Facility — The slow, non-equilibrium, dynamics in low-concentration (particle volume fraction Φ ≈ 20 %) depletion gels consisting of colloid-polymer mixtures was studied using X-ray photon correlation spectroscopy. In some recent work (A. Flerasu et al. PRE 76, 010401(R), 2007) we have shown that towards full aging, the intermediate scattering functions are well described by compressed exponential decays, indicating a form of “jamming” in the system which occurs even on length scales smaller than the particle radius. Here we extend these results by probing samples with different interaction potentials (tuned by the polymer concentration) and by characterizing the dynamical heterogeneities in these soft gels. We will also show first results on the formation of the gels in shear flow that were obtained using a combination of X-ray, direct observation, and co-flow mixing techniques.

K1.00283 Exceptionally stable organic glasses: a molecular view of the glass-to-liquid transformation, STEPHEN SWALLEN, KENNETH KEARNS, MARK EDGER, University of Wisconsin-Madison — Exceptionally stable organic glasses have been prepared by physical vapor deposition. Substrate temperature and deposition rate have been found to determine the degree of stabilization. When optimized, these factors allow the production of films with very slow kinetics and up to 2% more dense than the ordinary glass. This is as dense as the estimated density of the equilibrium supercooled liquid at Tg – 50 K. Translational motion, density and surface mobility were measured in films vapor deposited at a range of temperatures from Tg down to Tg – 150 K. Stable films can be superheated well above Tg, and the very slow relaxation rates allow the investigation of the glass-to-liquid “melting” transition. Results suggest this process occurs by nucleation and growth, with regions of low viscosity liquid developing within the glassy matrix.

K1.00284 Unexpected long range order at the early stage of spinodal decomposition, LEOPOLDO R. GOMEZ, DANIEL A. VEGA, Department of Physics - Universidad Nacional del Sur - Argentina — During the early stage of spinodal decomposition most of the phase separating systems lead to the formation of incoherent structures with small-range orientational and translational order. In this work we found that in the region near below the spinodal line two-dimensional systems with competing interactions can form hexagonal structures with long-range order. As a consequence of the strong mode selectivity, a network of density scars with large density fluctuations is formed at the early stage of the process of phase separation. The points of ramification of this network of scars act like nucleation centers of a hexagonal phase and ultimately define the domain structure, correlation length and statistical properties of the topological defects.

K1.00285 Nonequilibrium Assembly of Polymers and Quantum Dots from a Confined Geometry, ZHIQUN LIN, SUCK WON HONG, JUN XU, MYUNGHWAN BYUN, Iowa State University — Dissipative structures, such as scanned probe microscopy. We will address the relaxation dynamics in hydrogen-bonded super-cooled liquids near (but above) the glass transition, measured via Broad-Band Dielectric Spectroscopy (BDS). We propose a theory based on decomposing the relaxation of the macroscopic dipole moment into contributions from hydrogen bonded clusters of molecules. We discuss the statistical mechanics of the super-cooled liquid and with a theoretical estimate of the relaxation time of each cluster we provide predictions for the real and imaginary part of the frequency dependent dielectric response. Using glycerol as a particular example we demonstrate quantitative correspondence between theory and experiments. The theory also demonstrates that the ε peak and the “excess wing” stem from the same physics in this material.

K1.00286 Quantitative analysis of buried structures in polymer, nanoparticles and their nanocomposites by GISAXS, ZHANG JIANG, XUEFA LI, DONG RYEOL LEE, MICHAEL SPRUNG, JIN WANG, X-ray Science Division, Argonne National Laboratory — Grazing incident small-angle x-ray scattering (GISAXS) is a powerful and rapidly developing technique for the characterization of nanoscopic morphology and structures at surfaces. However, due to complicated data analysis involving distorted wave Born approximation (DWBA), most of the quantitative analysis nowadays is carried out only on surface structures. When combined with x-ray resonant-enhanced geometry, GISAXS can be extended to measure the buried structures in 3D polymer, nanoparticles and their nanocomposite thin films. In the current work, a more comprehensive approach is developed in order to extract in-plane structures as well as their depth-dependence within thin films, which cannot be readily accessible using conventional techniques, such as scanned probe microscopy.

1 This work and the use of the Advanced Photon Source are supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357
K1.00287 Self-Assembled Arrays of Non-Coalescent Water Drops, VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA 30332 — Condensation figures form over polymer dissolved in volatile solvent exposed to a stream of moist air. These patterns are hexagonally symmetric and they comprise of non-coalescent and nearly monodisperse water drops. Typical condensation figures have a range of drop sizes, resulting from the nucleation, growth and coalescence of different generations of water drops. In this study, we image the pattern formation over evaporating polymer solutions. We observe that rafts of growing drops evolve into a highly organized two dimensional lattice, which eventually evaporate away as well, templating ordered arrays of holes in polymer films. We derive the analytical and modeling framework for determining the key kinetic parameters that control the typical length scales and timescales of droplet growth, non-coalescence and assembly.

K1.00288 Equilibrium Switching: Nucleosomes and Transmembrane Proteins, DAVID SCHWAB, KARIM WAHBA, ROBIN BRUINSMA, Dept. of Physics and Astronomy, UCLA — The problem of placing rods on a line is an old problem in statistical mechanics. It has recently found applications in biology in the context of nucleosome positioning and transmembrane helix prediction. In both of these problems, the underlying lattice possesses a heterogeneous energy landscape, making the problem nontrivial. We explain the relative ease of helix prediction over nucleosome positioning as due to the existence of “switching” regions, i.e. a ground state density profile that deviates from that formed by successively occupying the lowest available energy minima. We illustrate the concept with a simple disorder systems model that can be solved exactly and discuss the functional implications for both transmembrane proteins and nucleosomes.

K1.00289 Flow through a reconstituted marine quartz sediment by an interacting lattice gas simulation, ALLEN REED, Naval Research Laboratory, EDWARD BRAITHWAITE, JOE GETTRUST, Naval Research Laboratory, RAS PANDEY, Naval Research Laboratory and University of Southern Mississippi — Regions of a reconstituted cylinder of quartz sediment (5.9 cm diameter x 13 cm long) from the Northern Gulf of Mexico were sub-sampled as 6.5 mm diameter cylinders. Images of sub-samples were made from x-ray micro-focus computed tomography data at 11 micron resolution. Using a coarse-grained approximation, each sample image is represented by a cubic lattice (100³ voxels). Fluid, a pool of particles at the lattice base supplies fluid-particles flows against gravity to the sink at the top of the lattice. In addition to the concentration gradient, an external pressure bias, similar to a hydraulic head drives the mobile particles upward against gravity. Particles are allowed to execute stochastic motion by a Metropolis algorithm. The porous medium is generated by a random distribution of barriers on a three dimensional lattice with a slit across the center. Interacting particles enter the lattice from the source and execute their stochastic motion with the Metropolis algorithm, and are driven by their concentration gradient and a pressure bias against gravity. Density and mobility profiles of particles in steady-state are studied as a function of pressure bias. A large fraction of particles flows through the slit with a relatively uniform dispersion in the surrounding porous regions in absence of the bias. Increasing the bias introduces long-range correlations among the constituents resulting in larger density further away from the slit. Effects of the size of the slit’s width on the density profile of particles and their mobility are also examined.

K1.00290 Distribution of self-organizing driven particles and their mobility around a slit in porous media, JOE GETTRUST, Naval Research Laboratory, RAS PANDEY, University of Southern Mississippi — Self-organizing structures and mobility profiles of a mixture of immiscible driven particles (A, B with molecular weights $M_A$, $M_B$) through a porous medium are examined by an interacting lattice computer simulation. The porous medium is generated by a random distribution of barriers on a three dimensional lattice with a slit across the center. Interacting particles enter the lattice from the source and execute their stochastic motion with the Metropolis algorithm, and are driven by their concentration gradient and a pressure bias against gravity. Density and mobility profiles of particles in steady-state are studied as a function of pressure bias. A large fraction of particles flows through the slit with a relatively uniform dispersion in the surrounding porous regions in absence of the bias. Increasing the bias introduces long-range correlations among the constituents resulting in larger density further away from the slit. Effects of the size of the slit’s width on the density profile of particles and their mobility are also examined.

K1.00291 Pair diffusion in quasi-one- and quasi-two-dimensional binary colloid suspensions, Binhua Lin, David Valley, Stuart A. Rice, Hau My Ho, School of Polymer, Textile and Fiber Engineering, University of Southern Mississippi — We report the results of experimental determinations of the triplet correlation functions of quasi-one-dimensional (q1D) and quasi-two-dimensional (q2D) binary colloid suspensions. The new results extend the findings of similar studies of one-component q1D and q2D colloid suspensions. Our principal new finding is that the presence of the smaller diameter component can destroy the oscillatory structure of the separation dependence of the q2D relative pair diffusion coefficient of the large particles even though the oscillatory character of the large particle equilibrium pair correlation function remains prominent, and that no such effect occurs with the q1D suspension. An interpretation of these results is proposed.

K1.00292 Three-particle correlation functions of quasi-two dimensional one-component and binary colloid suspensions, Binhua Lin, Hau My Ho, Stuart A. Rice, University of Chicago — We report the results of experimental determinations of the triplet correlation functions of quasi-two-dimensional one-component and binary colloid suspensions in which the colloid-colloid interaction is short ranged. The suspensions studied range in density from modestly dilute to solid. The triplet correlation function of the one-component colloid system reveals extensive ordering deep in the liquid phase. At the same density the ordering of the larger diameter component in a binary colloid system is greatly diminished by a very small amount of the smaller diameter component. The possible utilization of information contained in the triplet correlation function in the theory of melting of a quasi-two-dimensional system is briefly discussed.

K1.00293 Rotational Diffusion of Colloidal Clusters, Jakub Otwinowski, Kazem Edmond, Ken Desmond, Eric R. Weeks, Emory University — We synthesize fluorescent PMMA particles and form them into clusters of several particles. We separate the clusters and make dilute suspensions of identical clusters in an index and density matched solvent. We scan the suspensions with a high-speed confocal microscope in 3D over time. For each cluster we determine the position and orientation with modified particle tracking software, and we follow the translational and rotational motion in time. The diffusion coefficients for translational and rotational motion agree with the Stokes-Einstein and the Stokes-Einstein-Debye relations.

K1.00294 DNA Linker Mediated Crystallization of Nanocolloids, Huiming Xiong, Brookhaven National Laboratory, Daniel Van der Lelei, Oleg Gang — Biofunctionalized nanocolloids offer a promising platform for creation of novel materials using bio-addressable interactions. Crystalline phases are of especial interest for the development of novel functional structures. We demonstrate that crystallization of nanocolloids can be achieved via hybridization of dispersed non-complementary single stranded DNA capped colloids with flexible single-stranded linker DNA. The crystalline structure belongs to body central cubic lattice and exhibits large thermal expansion. The evolution of the structure has been studied in details using in-situ small angle x-ray scattering. The formation of crystalline structures and reduced metastability are observed for systems with longer DNA linkers.

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1This work has been supported by the NSF CTS-021174 and CHE-9977841, the Israel Science Foundation 77/03 , the NSF funded MRSEC laboratory at The University of Chicago, and by a Senior Mentor Grant to S.A.R. from the Dreyfus Foundation.

3This research was supported by a grant from the NSF CHE-9977841 and by the MRSEC Laboratory at The University of Chicago.

3Research carried out at the Center for Functional Nanomaterials and the National Synchrotron Light Source, was supported by the U. S. DOE Office of Science and Office of Basic Energy Sciences.
K1.00295 Translation-rotation coupling in concentrated colloidal suspensions, MINSU KIM, Physics, UIUC, STEPHEN ANTHONY, Chemistry, UIUC, STEVE GRANICK, material science and engineering, UIUC — Single-particle tracking has been used to contrast translational and rotational diffusion in monodisperse colloidal suspensions. Visualization of angular motion reveals that rotation has different properties from translation. Collective motions of particles lead to subdiffusive rotation. Deviations from Fickian motion increase as the volume fraction increases above 50%. Translational and rotational coupling of a single particle is measured directly for the first time and its dependence on the volume fraction is discussed.

K1.00296 Large Scale Computer Simulation of Erythrocyte Membranes with Explicit Cytoskeleton†, CAMERON HARVEY, JOEL REVALEE, MOHAMED LARADJI, University of Memphis, P.B SUNIL KUMAR, IIT-Madras, Chennai, India — The erythrocyte membrane is composed essentially of a self-assembled lipid bilayer and a polymerized protein meshwork, referred to as the cytoskeleton. For the erythrocyte, the polymer meshwork is composed of spectrin and anchored to the bilayer through specialized proteins. In this investigation we extended a coarse-grained model of self-assembled lipid membranes, recently developed by us, to account for the cytoskeleton. Simulation of bilayer patches, with dimensions about 0.5 μm × 0.5 μm, were performed to investigate the effects of the cytoskeleton on the membrane elastic properties. The bending modulus and surface tension are extracted from the spectra of the out-of-plane thermal undulations of the membrane. Using Monte Carlo, we also extracted the compression and shear moduli. Preliminary findings suggest a measurable effect in thermal undulations resulting from the introduction of the cytoskeleton.

K1.00297 QUANTUM INFORMATION, CONCEPTS, AND COMPUTATION II —

K1.00298 ABSTRACT WITHDRAWN —

K1.00299 Transconductance of a double quantum dot system coupled to a microcavity, VIJAY KASISOMAYAJULA, PETER BONANNO, ONOFRIO RUSSO, New Jersey Institute of Technology — The transconductance of a double quantum dot system in the coulomb blockade regime for single spin 1/2 electrons on each dot mutually coupled by an exchange interaction has been studied. We investigate the effect of this system when coupled to a microcavity and determine conditions for the external potential on each of the dots. The significant peaking in the transconductance as found without cavity mode coupling, is due to a large degree on the potential of each dot. The electron spins on each of the quantum dots are responsible for the strong mutual interaction but, also these spins result in only weak coupling to the adjacent leads. The weak Kondo condition, however is responsible for the enhanced transconductance. The addition of the dominant modes of a strongly coupled microcavity and its effect on the transconductance are discussed for differing potentials and spacing between the dots, and for some conditions result in an enhanced transconductance. L. V. Koerten, P. Wolfe, PRL 99, 036807(2007)

K1.00300 The role of state preparation in quantum process tomography, KAVAN MODI, AKI-MENG KUAH, CESAR RODRIGUEZ-ROSAIRO, GEORGE SUDARSHAN, The University of Texas at Austin — We study the effects of preparation of input states in a quantum tomography experiment. We study two preparation procedures, stochastic preparation and preparation by measurements. It turns out that the stochastic preparation procedure yields linear process maps, while the results obtained from an open system that is initially prepared using von Neumann measurements is shown to be non-linear, and can only be consistently described by a bilinear process map. A new process tomography recipe is derived for preparation by measurement for qubits. The difference between preparing states for an experiment by measurement and by stochastic process is analyzed.

K1.00301 Quantifying the role of interference in quantum information processing, DANIEL BRAUN, BERTRAND GEORGET, LUDOVIC ARNAUD, University Paul Sabatier Toulouse — We present a quantitative measure of interference, applicable to any quantum mechanical process in a finite dimensional Hilbert space, and use it to examine the role that interference plays in various quantum algorithms and other quantum information theoretical tasks. We present results for the amount of interference in both Grover’s search and Shor’s factoring algorithms, and on how interference correlates with success probability in the case of disturbances of these algorithms through static or random unitary errors, or decoherence through bit-flips and spin flips [1]. We have also studied the statistics of interference in random quantum algorithms, both using well known random matrix ensembles (CUE, the circular unitary ensemble, and HOE, the Haar orthogonal ensemble), as well as recently introduced random circuit ensembles. We show that interference distributions in the random circuit ensembles converge rapidly (i.e. exponentially, or even in a Gaussian fashion) towards the universal interference distributions of CUE and HOE, which predict close to maximum interference with very high probability for a randomly picked quantum algorithm [2].


K1.00302 Resonant activation and multi-junction switching characteristics of Bi-2212 intrinsic Josephson junctions, NOBUHIRO KITABATAKE, RIEC, Tohoku Univ., KUNIHIRO INOMATA, RIKEN, SHIGEO SATO, RIEC, Tohoku Univ., MITSUNAGA KINJO, Department of Electrical and Electronic Engineering, Univ. of the Ryukyus, HUBING WANG, TAKESHI HATANO, NIMS, KOJI NAKAJIMA, RIEC, Tohoku Univ. — Bi-2212 intrinsic Josephson junctions (IJJs) are expected to be applied to a superconducting qubit. We have studied quantum behavior of two different types of Bi-2212 IJJs, one is fabricated by FIB etching [2,3] and the other is fabricated by Double Side Etching Method (DSEM) [4]. In this report, we show their multi-junction switching properties with or without microwave irradiation. The experimental results indicate that the couplings between junctions change according to the sample fabrication process. [1] K.Inomata et al., Phys. Rev. Lett. 95, 107005 (2005) [2] S.-J.Kim et al., Appl. Phys. Lett. 74,1156 (1999) [3] Yu.I.Latyshev et. al., JETP Lett. 69, 84 (1999) [4] H.B.Wang et al., Appl. Phys. Lett. 78, 4010 (2001)

K1.00303 Macroscopic Resonant Tunneling Above the Crossover Temperature in a rf SQUID†, LUIGI LONGOBARDI, DOUGLAS BENNETT, VIJAY PATEL, JAMES LÜKENS, Stony Brook University, Department of Physics and Astronomy — We report studies of macroscopic resonant tunneling (MRT) between fluxoid states in an rf-SQUID qubit as function of temperature. The measured tunneling rates as a function of bias exhibit evidence of energy level quantization up to a temperature (900 mK) well above the crossover temperature (Tc) between the quantum and the thermal regime. The data agree with the level structure calculated using independently measured circuit parameters. The MRT is a useful probe of decoherence-inducing noise in the rf SQUID since the measurements are much simpler and give values for flux noise equal to those obtained from Tz.

†This work has been supported in part by NSF and by AFOSR and NSA through a DURINT program.

K1.00304 Universal quantum degeneracy point for solid-state qubits†, L. TIAN, Department of Applied Physics and E. L. GinZton Laboratory, Stanford University, Stanford, CA 94305 — When operated at the quantum degeneracy point, the so called “sweet spot”, solid-state qubits can be protected from the first order decoherence of low-frequency noise in the off-diagonal coupling. Here, we show that a quantum degeneracy point can also be found for low-frequency noise in the diagonal coupling in an encoded-qubit scheme. We also study the protocols for implementing one and two bit quantum logic gates and the effects of circuit imperfection on this scheme. A practical system to realize this scheme with superconducting qubits is then presented.

†This work is supported by the Karel Urbanek Fellowship and the SORST program of JST.
K1.00305 SURFACES, INTERFACES AND THIN FILMS —

K1.00306 Diffusion Prefactors and Vibrational Entropic Contributions for small Cu and Ag clusters on Cu(111) and Ag(111) 1. HANHAND YILDIRIM, ABDKADER KARA, TALAT S. RAHMAN, Department of Physics, University of Central Florida — In examination of the diffusion energetics and dynamics of small 2D Ag and Cu clusters on Ag(111) and Cu(111) we found the results for the 7-atom cluster to be particularly interesting. In particular the diffusion pre-exponential factor for the Cu clusters on Ag(111) is found to be one order of magnitude larger than that for the homo-systems; Cu cluster on Cu(111) and Ag cluster on Ag(111). Analysis of the vibrational entropic contributions to the system free energy points to the subtle differences in the three cases and the significant contribution of the substrate atoms that lie in the vicinity of the diffusing islands. We trace the differences in the results for the 7-atom cluster from those for smaller sized ones to the nature of the cluster-substrate interactions. The vibrational dynamics and energetics of the systems are obtained using ab initio electronic structure calculations (density functional theory) and compared to those obtained using many body interaction potentials.

1This work was supported in part by NSF-ITR 0428826 and DOE grant DE-FG02-03ER46354.

K1.00307 Magnetic studies on thin films of iron oxides, JAYA OSORIO, JUAN URIBE, CESAR BARRER, DORIS GIRATA, ALVARO MORALES, Universidad de Antioquia, AXEL HOFFMANN, Argonne National Laboratory, RAMON GANCEDO, CSIC, ESTADO SOLIDO TEAM, MATERIALS SCIENCE DIVISION TEAM, INSTITUTO ROCASOLANO TEAM — We have grown hematite (α-Fe₂O₃) thin films on stainless steel and silicon dioxide (SiO₂) substrates and magnetite (Fe₃O₄) thin films on silicon substrates by RF magnetron sputtering process. Conversion Electron Mössbauer (CEM) spectra of these films exhibit hyperfine parameter values which are characteristic of these iron oxides. Magnetization measurements parallel to the plane of the film as a function of temperature, M(T), were done at a constant field of 1 kOe to α-Fe₂O₃ films and at 200 Oe to Fe₃O₄ films. The M(T) curve of the α-Fe₂O₃ film showed a linear increasing of magnetization from 5 K to 160 K, related with the Morin transition. While the temperature of the Fe₃O₄ film is decreased, a sharp decrease in magnetization is observed at 123 K, associated to the Verwey transition. We carried out measurements of magnetization as a function of applied magnetic field, the loops of α-Fe₂O₃ film exhibits hysteresis which is related to their weakly ferromagnetic behavior and the loops of the Fe₃O₄ film at 300 and 110 K show a magnetic value around 5 memu at 3 Koe in the curves.

K1.00308 Far-from-equilibrium Ag-Cu thin-films on Cu(100) and Ag(100) substrates, ANTONIO CADILHE, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; GCCP-Centro de Fisica da Universidade do Minho, 4710 Braga, Portugal, NUNO A.M. ARAUJO, GCCP-Centro de Fisica da Universidade do Minho, 4710 Braga, Portugal; T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, A.F. VOTER, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — We study the dynamics of multilayer, heteroepitaxial deposition of mixed incoming fluxes of Ag and Cu atoms and the corresponding post-deposition relaxation on Ag (100) and Cu (100) substrates. To this end, we carried out extensive temperature accelerated dynamics (TAD) simulations at different substrate temperatures to characterize the morphology of the resulting films. Depending on the flux of impinging atoms, the number of layers, and the substrate temperature, the system can exhibit kinetically trapped, far-from-equilibrium configurations. Complex multi-adatom moves, not usually accounted for in regular Monte Carlo simulations, have a non-trivial relevance in the dynamics.

K1.00309 Chemical and structural dynamical equilibrium in bimetallic nanoclusters, JÉRÔME CREUZE, LEMHE/ICMOMO, UMR 8182, Université Paris Sud-XI, Bat. 410, F91405 Orsay cedex, France, LAURE DELFOUR, BERNARD LEGRAND, SRMP-DMN, CEA Saclay, F91191 Gif-Sur-Yvette cedex, France — Coupling the surface and finite-system thermodynamics is a challenging key point in modeling bimetallic clusters. This is particularly crucial when the alloy surfaces undergo first-order phase transitions. In this context, we have investigated the segregation of Ag atoms in the substructures (Ag₇O₇) and Ag₃O₃ by using N-body interaction potentials and the Monte Carlo method. The (111) and (100) surfaces of Cu-Ag alloys are known to exhibit first-order phase transitions coupling a jump in the surface concentration and structural rearrangements. For the Wulff polyhedron of 405 atoms, these phase transitions are replaced by a dynamical equilibrium (DE) in phase space. For the (100) facets, this DE affects both the composition and the structure of the facets. Furthermore, all the (100) facets are correlated during the DE, due to atomic relaxations which affect also the core region of the nanocluster. For the (111) facets, the DE concerns only the composition of the facets, the atomic structure remaining unchanged. Consequently, the (111) facets are not correlated each other, indicating that pure Ag and pure Cu (111) facets can be observed in a given nanocluster. These simulations allow us to propose a surface phase diagram for the studied Wulff polyhedron.

K1.00310 Mechano-Chemical Stability of Gold Nanoparticles Coated with Alkanethiolate SAMs1, BRIAN HENZ, U.S. Army Research Laboratory, TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — Molecular dynamics simulations are used to probe the structure and stability of alkanethiolate self-assembled monolayers (SAMs) on gold nanoparticles. We have observed that the surface of gold nanoparticles become highly corrugated by the adsorption of the SAMs. Furthermore, as the temperature is increased, the SAMs dissolve into the gold nanoparticle, creating a liquid mixture at temperatures much lower than the melting temperature of the gold nanoparticle. By analyzing the mechanical and chemical properties of gold nanoparticles at temperatures below the melting point of gold, with different SAM chain lengths and surface coverage properties, we have determined that the system is metastable. The model and computational results that provide support for this hypothesis are presented.

1NSF, ARL

K1.00311 Morphology and Growth Dynamics of Buckling Polymer Surfaces, DEREK BREID, Dept. of Polymer Science and Engineering - University of Massachusetts, ALFRED CROSBY, Dept. of Polymer Science and Engineering, University of Massachusetts — Surface buckling is an expected response of a polymer surface when an applied in-plane stress exceeds a material-defined critical stress. This onset of a prescribed surface structure has been gaining increasing attention over the last decade towards applications as diverse as enhanced adhesion and flexible circuitry. However, the majority of research has been performed for systems subjected to stresses well above their critical buckling stress. Here, we highlight recent experiments that characterize the buckle morphology and dynamic buckling behavior of an oxidized PDMS surface swollen with solvent vapor. At low stresses, we observe the spontaneous formation of hexagonally packed microlens arrays not predicted by current buckling theory. These structures coalesce at higher stresses into predicted morphologies. This understanding provides new routes for the controlled formation of surface patterns with complex arrangements and geometries.
K1.00312 Preparation and Characterization of Ta$_2$O$_5$–CeO$_2$ Films, DURSEN SAYGIN HINCZEWSKI, Istanbul Technical University, I.T.U., KENAN KOC, Yildiz Technical Univ., IDRIS SORAR, I.T.U., MICHAEL HINCZEWSKI, TUBITAK Bosphorus Univ, Feza Gursey Institute, FATMA Z. TEPEHAN, I.T.U., GALIP G. TEPEHAN, Kadir Has Univ. — Ta$_2$O$_5$ films have been widely studied due to their chemical and thermal stability, high dielectric constant and refractive index. It is known, for certain composites of Ta$_2$O$_5$–TiO$_2$, Ta$_2$O$_5$–Al$_2$O$_3$, and Ta$_2$O$_5$–ZrO$_2$ polycrystalline ceramics, that there is a significant increase in the dielectric constant compared to pure Ta$_2$O$_5$; this has stimulated research of doped thin films of Ta$_2$O$_5$. In this study [1], the sol-gel spin coating method has been used to make Ta$_2$O$_5$–CeO$_2$ thin films. These films have been prepared in various composition ratios to observe changes in their surface morphology, optical and structural properties. Reflectance and transmittance spectra were collected in the spectral range of 300-1000 nm, and were accurately fit using the Tauc-Lorentz model. Film thicknesses, refractive indices, absorption coefficients, and optical band gaps were extracted from the theoretical fit. The highest refractive index value was found at 5% CeO$_2$-doping. The structure of the films was characterized by XRD and FTIR spectrometry, while the surface morphology was examined through AFM. [1] D. Saygin-Hinczewski, K. Koc, I. Sorar, M. Hinczewski, F.Z. Tepehan, and G.G. Tepehan, Sol. Energy Mater. Sol. Cells 91, 1726 (2007).

K1.00313 On x-ray scattering by solitons in systems of adsorbed atoms, IRINA BARIAKHTAR, Boston College, VICTOR BARYAKHTAR, Institute of Magnetism, Ukraine — The cross section for scattering of x-rays by solitons is calculated. The authors consider solitons corresponding to the formation of a kink in a system of adatoms on the surface of a substrate, or a crowdion in a chain of adatoms in crystals described by the sine-Gordon equation, and also solitons in a bound electron-phonon quasi-one-dimensional molecular chain. It is shown that study of the x-ray scattering provides for the possibility to gather information on the static and dynamic properties of the solitons.

K1.00314 On electromagnetic wave propagation in systems of adsorbed monolayers, IRINA BARIAKHTAR, Boston College, VALERI LOZOVSKI, National University of Kiev, Ukraine — Taking into account the discrete nature of the adsorbed layer, the authors study electromagnetic waves in the system of insulating substrate with the monolayer of adsorbed molecules. Calculated are the dispersion relations of the excitations with s- and p- polarizations localized at the adsorbed layer. To obtain the linear response of such systems, Green’s function approach was undertaken. The susceptibility tensor of the system is expressed in terms of Green’s function, and the pole structure of the susceptibility is investigated.

K1.00315 Complex electronic interference effects in Ag films on Ge(111), YANG LIU, NATHAN SPEER, University of Illinois at Urbana-Champaign, SHU TANG, National Tsing Hua University, THOMAS MILLER, TAI CHIANG, University of Illinois at Urbana-Champaign — We have performed a 3-D mapping by angle-resolved photoemission of the electronic structure of atomically uniform Ag thin films grown on Ge(111). Electrons in the Ag film with energies within the absolute gap of Ge are fully confined, forming quantum well states, while electrons with energies outside this gap form quantum well resonances. In addition to these features, our results show complex interference patterns from which can be attributed to umklapp processes at the interface. The lattice mismatch between Ag and Ge creates an incommensurate interface, which introduces multiple periodicities, resulting in a rich electronic structure. We have performed a detailed numerical analysis of the experimental results, and the interaction parameters, related to the interfacial potential modulation, are extracted.

K1.00316 Effects of Energetic Particles on Friction Behavior of Diamond-like Carbon, KE WANG, HONG LIANG, Texas A&M University, JEAN MICHEL MARTIN, THIERRY LE M OGNE, — This research investigates the failure mechanisms of damages induced by interactions of energetic particles and a diamond-like carbon (DLC) film. Experimental approaches include using an ultra-high vacuum tribometer with attached spectroscopic analysis techniques to generate those particles and conduct in-situ tribological testing. Analytically, using multiple-peaks deconvolution to analyze carbon 1s X-ray photoelectron spectroscopy (XPS) results, the bonding information of C atoms on the surface of DLC film has been extracted. Comparing with friction test results, it is found that the frictional behavior of DLC film (after the reaction with energetic particles) strongly depends on the ratio between sp3 and sp2 hybridization of C atoms on the surface.

K1.00317 Nonextensivity in Magnetic Systems, IVAN OLIVEIRA, DIOGO PINTO SOARES, ROBERTO SARTHOUR, Brazilian Center for Research in Physics, MARIO REIS, Ciceco - Aveiro University — Nonextensive statistics has been successfully applied to different areas of physics, whenever long-range correlations, fractality, inhomogeneity or long memory time are present. Nonextensive thermodynamics is derived from the definition of nonextensive entropy: \[ S_q = k \left( 1 - \sum_i p_i^q \right)/(q-1) \], where \( p_i \) are probabilities and \( q \) is the so-called entropic index. From this definition one obtains the q-density matrix, \( \rho^q \), and, from it, thermodynamically related quantities. In condensed matter, strong correlated systems are good candidates to be studied in the nonextensive approach. The paper is an overview of the results obtained in this field of research. A variety of inhomogeneous media using the nonextensive approach.

K1.00318 Low temperature metamagnetic transitions in single crystal ErNi$_2$B$_2$C: torque magnetometry study, DONALD NAUGLE, K.D.D. RATHNAYAKA, Texas A&M University, BORIS BELEVTSOEV, B. Verkin Institute for Low Temperature Physics and Engineering, SUNG-IK LEE, Pohang University of Science and Technology — The phase diagram of metamagnetic transitions in single-crystal rare-earth nickel borocarbide ErNi$_2$B$_2$C has been determined at 1.9 K with a Quantum Design torque magnetometer. The critical fields of the transitions depend crucially on the angle between applied field and the easy axis [100] in the a-b-plane. Torque measurements have been made while sweeping the magnitude of the magnetic field at a constant angular direction (parallel to basal tetragonal a-b-planes) over an angular range greater than two quadrants. Sequences of metamagnetic transitions with increasing field differ for the fields along (or close enough to) the easy [100] axis from those near the hard [110] axis. These torque measurements reveal new metamagnetic states in ErNi$_2$B$_2$C which were not apparent in previous longitudinal-magnetization and neutron studies. Their nature is considered and clarified. In the low-field range influences of superconductivity are observed and interpreted. 

K1.00319 Phase diagram of Na$_1$-xCaxV2O4 compounds synthesized at high pressure, TAMAS VARGA, JOHN MITCHELL, Argonne Natl Lab, KAZUNARI YAMAURA, DAVID MANDRUS, Oak Ridge Natl Lab, JUN WANG, Argonne Natl Lab — Ambient pressure CaV2O4 and high-pressure Na$_1$V2O4 crystalize in the CaFe2O4 structure type containing double chains of edge-sharing VO6 octahedra. Recent measurements on Na$_2$V2O4 reveal low-dimensional metallicity and evidence of half-metallic ferromagnetism. In contrast, Ca$_2$V2O4 is an antiferromagnetic insulator. To explore the evolution of these ground-state behaviors, we have prepared a series of Ca-doped Na$_2$V2O4 compounds with the formula Na$_{1-x}$CaxV2O4 (x=0-1) using high-pressure synthesis. The lattice parameters of Na$_{1-x}$CaxV2O4 samples change with nominal x according to Vegard’s law. The metallic state in Na$_2$V2O4 is dramatically altered by Ca doping. Samples with higher Ca concentrations (x=0.6-0.8) exhibit a metal-insulator transition around 150 K. Samples at the Na end (x=0-0.2) show a broad antiferromagnetic transition in the 120-160 K range in accordance with earlier reports. With increased Ca doping, the antiferromagnetic transition is suppressed to ∼70 K at the Ca-endmember. Transport measurements show an insulator-metal transition at x∼0.4. Comparison to existing studies at the Ca- and Na-rich ends will be discussed along with a schematic (T-x) phase diagram for the Na$_{1-x}$CaxV2O4.
This work was supported in part by National Natural Science Foundation of China (Grant No.50272009, 50572024), and NSF-PREM program (Grant No. 0351449).
K1.00328 Structural and physical properties of Fe-doped LiMn\textsubscript{2}O\textsubscript{4} oxides\textsuperscript{1}, YANG LI, Department of Engineering Science and Materials, University of Puerto Rico at Mayaguez, PR 00681, USA, BOYU MA, NING CHEN, YANG LIU, WEIPENG WANG, AIHUA WANG, XINGQIAO MA, GUOHUI CAO, Department of Physics, University of Science and Technology Beijing, 100083, China — A joint experimental and theoretical study of the physical property and electronic structures in Fe-doped LiMn\textsubscript{2}O\textsubscript{4} has been performed. The samples with pure phase are prepared by the solid reaction. The X-ray diffraction refinement and SEM analysis show that Fe enters lattice to occupy Mn site. The physical property measurements indicate that Fe doping results in modification of microstructure. The physical properties heavily depend on Fe-doping concentration. The first-principles simulations show that charge ordering and magnetic ordering occur in Fe-doped samples. The electron increasing in the system results in carrier concentration changing.

\textsuperscript{1}This work was supported in part by National Natural Science Foundation of Beijing (Grant No. 1072007), and National Science Foundation PREM program (Grant No. 0351449)

K1.00329 Small Angle X-ray Scattering of Self-assembling Systems Composed of Phosphocholine Lipids and Dendrimers, DEREK DORMAN, PAUL RUSSO, Louisiana State University — Polypropyleneimine tetraamine (DAB-Am) and 1-directional arboral dendrimers have been studied in different molar concentrations with 1,2-Dioleoyl-sn-Glycero-3-phosphocholine (DOPC). One-directional arborals are amphiphilic dendrimers with hydrophilic head group composed of 9 hydroxyl groups and a short alkyl chain for the hydrophobic tail. Film and liposome shell thickness was determined using small angle x-ray scattering beamline at the Center for Advanced Microstructures and Devices at Louisiana State University.

K1.00330 Conformational Space of Hydroxyacetone Studied by Matrix-Isolation FTIR Spectroscopy and Quantum Chemical Methods\textsuperscript{1}, A. SHARMA, I. REVA, R. FAUSTO, University of Coimbra, Portugal — The matrix-isolation FTIR spectrum of hydroxyacetone monomers isolated in Ar matrix at 12K was studied. Interpretation of the experiment was aided by MP2 and DFT calculations at the 6-311++G(d,p) level. A 2D potential energy surface, in the space of OCCO and HOCC dihedral angles, revealed 4 non-equivalent minima, C\textsubscript{c}, T\textsubscript{g}, T\textsubscript{t} and C\textsubscript{t}. The energy barriers for T\textsubscript{g}→T\textsubscript{t} and C\textsubscript{t}→C\textsubscript{c} conversions (0.7 kJ/mol both) were found to be below the zero-point vibrational level associated with the isomerization coordinate of the higher energy form in each pair (T\textsubscript{g} and C\textsubscript{t}). Then, only C\textsubscript{c} and T\textsubscript{t} forms have physical meaning. In accord with the relative energy calculated for T\textsubscript{t} (>11 kJ/mol), its estimated population in gas phase at 298K is only 1%. Indeed, only C\textsubscript{c} form was experimentally detected. Its characterization included the full interpretation of the vibrational spectrum and the calculation of the NMR spectra of the compound in different media.

\textsuperscript{1}This work was supported by Portuguese Science Foundation (FCT) Grant n SFRH/BPD/31840/2006 and Research Projects POCI/QUI/58937/2004 and POCI/QUI/59019/2004.

K1.00331 Synthesis and characterization of size-selected Ag nanoparticles with icosahedral shape\textsuperscript{1}, MIGUEL GRACIA-PINILLA, EDUARDO PEREZ-TIJERINA, SERGIO MEJIA-ROSALES, Universidad Autonoma de Nuevo Leon, MIGUEL JOSE-YACAMAN, University of Texas at Austin — We report the synthesis of Ag nanoparticles, produced by the technique of Inert Gas Aggregation, which allows a very precise selection of the nanoparticle sizes and deviations. We found the optimal experimental conditions to synthesize nanoparticles of six different sizes: 1.3±0.24, 1.7±0.35, 2.5±0.44, 3.7±0.41, 4.5±0.88, and 5.5±0.24 nm. With this, we were able to investigate the dependence of the size of the nanoparticles on the synthesis parameters. Our data suggest that the aggregation of clusters (dimers, trimers, etc) inside of the nanocluster source is the predominant physical mechanism for the formation of the nanoparticles. In order to preserve their structural and morphological properties, the impact energy of the clusters landing into the substrate was controlled; the acceleration energy of the nanoparticles was around 0.1 eV/atom, assuring a deposition in a soft landing fashion. HRTEM and HAADF-STEM images showed that the particles were icosahedral.

\textsuperscript{1}This work was supported by CONACYT, (scholarship 207569).

K1.00332 Directed polymer in random media with a defect, JIN MIN KIM, JAE HWAN LEE, Soongsil University — We investigate a directed polymer in random media with an attractive defect at the center of the one dimensional substrate. Without the defect, end to end distance $\Delta x \sim x^{1/2}$ with $x = 2/3$ which is related to the value of the dynamic exponent in Kardar-Parisi-Zhang equation. When the defect strength $\epsilon$ is weak, its contribution to $\Delta x$ is negligible. If $\epsilon > \epsilon_c$, then $\Delta x$ becomes constant. This kind of transition is related to a queuing phenomena in the asymmetric simple exclusion process. Various critical exponents near the transition point are also discussed.

K1.00333 Thermal conductivity measurements of Bi\textsubscript{2}Te\textsubscript{3} nanowire arrays in anodic aluminum oxide template by 3$\omega$ method, PING-CHUNG LEE, CHENG-LUNG CHEN, MIN-NAN OU, YANG-YUAN CHEN, Institute of Physics, Academia Sinica — Bismuth telluride is a thermoelectric material which is famous for its high figure of merit $ZT \sim 1$. Theoretical predictions propose that the thermoelectric properties of nanowires could be greatly enhanced compared to its bulk form. We have prepared Anodic Aluminum Oxide (AAO) templates with 60 nm pore diameter, 80 $\mu$m thick and ~30% porosity, and synthesized bismuth telluride nanowire arrays into the AAO template by electrodeposition. The modified version of the 3$\omega$ slope method [1] was employed to measure the anisotropic thermal conductivity of the nanowire array in AAO template. This report presents the temperature dependent cross-plane (parallel to nanochannel) and in-plane (perpendicular to nanochannel) thermal conductivity of the nanowires. And estimate the thermal conductivity of bismuth telluride nanowire specifically by using a nanowire filling factor of ~30% in a temperature range of 80-300 K.


K1.00334 Theoretical Study on F atom diffusion on Si(111) surface, NARA JUN, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo, YUSUKE ASARI, National Institute for Materials Science, TAKAHIRO OHNO, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo — We studied diffusion mechanisms of fluorine atom adsorbed on Si(111) surface in a low coverage regime by means of the first-principles density functional calculation. Recent experiments found that the diffusion frequency of the fluorine atoms on Si(111)-(7x7) surface is very low and interestingly it is enhanced after the deposition of silicon atoms on the surface. While this measurement strongly suggests that the diffusing extra silicon atoms assist the fluorine migration, the mechanism has not been understood yet. We found that it is hard for F atoms to hop between surface Si atoms directly because of the strong Si-F bonding. Instead we suggest the SiF complex diffusion model, in which SiF bond is kept during diffusion. This model is also understood as the Si atom diffusion with carrying the F atom. This model, in which the activation energy is calculated to be 1.34 eV, can explain the experiment very well. This work was partly supported by RSS21 project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.
A setup for simultaneously measuring the thermopower and electrical conductivity of \(\mu\text{m}\)-thickness specimens, CHIH-TING CHEN, Institute of Physics, Academia Sinica, P.C. LEE, Y.Y. CHEN, SERGEY HARUTYUNYAN, INSTITUTE OF PHYSICS, ACADÉMIA SINICA TEAM — We report the concept and configuration of our new setup for measurement of thermopower and electrical conductivity for \(\mu\text{m}\)-thickness specimens, especially for thermoelectric materials. It is very difficult and tedious to accurately measure the thermopower for specimens with thickness less than \(\sim 100 \mu\text{m}\) due to the limitations of smallest size \(\sim 25 \mu\text{m}\) of thermocouples. Such are obvious when applied to the measurement of nanowire arrays and multilayer. In order to resolve these difficulties, we developed a new setup with integration of Pt-film thermometers and electrical electrodes on two sapphire chips used to clamp specimens with thickness \(\geq 40 \mu\text{m}\) and cross section \(2 \times 3 \text{ mm}^2\). Use this setup the thermopower and electrical conductivity can be measured simultaneously for temperature range 20-400 K. The advantages of the setup are (1) accuracy: the real temperatures of both sides of the sample can be obtained. (2) convenience for loading samples: just assemble the sample between the two microchips and make sure of a good thermal and electrical contacts. A Bi\(_2\)Te\(_3\) nanowire array in AAO template was tested, the thermopower \(\sim 50\text{\mu V}/\text{K}\) was measured for diameter \(60 \mu\text{m}\) of nanowires.

**K1.00336** SNS-Magnetism Reflectometer Initial Measurements, H. AMBAYE, R. GOYETTE, Oak Ridge National Lab-SNS, G. FELCHER, Argonne National Lab, A. PARIZZI, Oak Ridge National Lab-SNS, F. KLOSE, ANSTO — The SNS Magnetism Reflectometer is one of the first three operational SNS instruments. Its construction was completed in May 2006 and the first data sets were collected in July 2006, shortly after passing the instrument readiness safety review. The beamline commissioning proceeds in parallel to the power ramp up of the SNS accelerator. While the initial reflectivity measurements were taken with only 250 Watts of proton power, by mid November 2006 proton power had already increased to 60 kW, making the SNS the most intense pulsed neutron source on a per pulse basis and in August 2007 by running at 185kW became the most intense source in the world. In this presentation, initial commissioning results for the Magnetism Reflectometer, in particular beam intensity/divergence measurements, tests of the polarized neutron equipment (super mirror polarizer, large spin flippers) as well as transmission measurements of the bandwidth limiting chopper systems and some science reflectivity measurements will be presented. Reflectivity data for magnetic MgO and Si3Na/Mn multilayer will be discussed in this presentation. The magnetic MgO:N(2.2%) is a system that is doped with 2.2% Nitrogen there by introducing a local magnetic moment of about 8emu/cc. The SNS Magnetism Reflectometer on beamline 4A shares a common primary beam port and shutter with the SNS Liquids Reflectometer (BL4B) from which it is separated by 4.8˚ in horizontal angle. Individual secondary shutters allow operating the two instruments independently.

**K1.00337** Magnetic resonance force microscopy with two-dimensional spatial encoding, KAI W. EBERHARDT, URBAN MEIER, ANDREAS HUNKELER, BEAT H. MEIER, ETH Zurich — We demonstrate a novel method of creating Magnetic Resonance Force Microscopy (MRFM) images that eliminates the need to scan the probe-sample distance. Conventionally, scanning a magnetic tip over the sample in at least two dimensions is required for imaging with MRFM. At each position the signal from a different slice of the sample is acquired, where the slice is defined by the rf field and the ferromagnetic gradient tip geometry. An image can be reconstructed by deconvolving the shape of the slice from the data. The new method we demonstrate keeps the sample-tip distance constant and resolves the signal origin by spatial encoding with rf pulses. For spatial encoding in one dimension rf pulses are applied with a gradient field coil. These pulses produce a Fourier-encoding in the longitudinal magnetization. In the second dimension Hadamard encoding [1] is employed. 2D images of a patterned (NH\(_4\))\(_2\)SO\(_4\) crystal sample are reconstructed from the known field distributions with a resolution of 1 \(\mu\text{m}\) at room temperature. [1] K. W. Eberhardt et al., Phys. Rev. B 76: 180405 (2007)

**K1.00338** Optical and Transport Study of Nanocomposite Film of Polymer and PbS Quantum Dots, JIAN ZHANG, XIAOMEI JIANG, Department of Physics, University of South Florida — Optical studies have been done with nanocomposite of conjugated polymers with colloidal lead sulfide PbS quantum dots (QDs). Partial quenching of polymer photoluminescence by PbSe QDs showed the co-existence of energy and charge transfer within this system. Further investigation by means of cw spectroscopy (including photoluminescence action spectroscopy, photo-induced absorption spectroscopy and photoluminescence quantum efficiency) have been rendered for comprehensive study regarding photogenerated charge transfer. Transient transport and time of flight measurements have been employed to conduct mobility and recombination rate study of the same film. The size dependent optoelectronic properties were observed and explained by model fittings. Life time and activation energies were drawn from the fittings. Study also shows improvement on both optical absorption and charge transfer properties with QDs being treated with post-synthesis ligands exchange.

**K1.00339** Multiscale modeling of early stage growth of CNTs produced by a catalytic CVD process, JAMES ELLIOTT, University of Cambridge, YASUSHI SHIBUTA, University of Tokyo — The catalytic chemical vapour deposition process is a widely used method for the production of single and multi-wall carbon nanotubes (CNTs), but there remain many uncertainties concerning the precise synthesis mechanisms and the properties of the CNTs that can be produced. Hence, we have developed a parameterized mesoscale model to simulate the early stages of growth of CNTs, and used this to establish a connection between the carbon-catalyst interaction energy, carbon deposition rate and catalyst particle shape and size and the type of CNT produced. The interaction energies for the various components of the model were determined using molecular dynamics simulations [1] using potential functions previously derived from density functional calculations [2] for cobalt, iron and nickel catalyst particles interacting with carbon. We present results from simulations for the different surface energies of the carbon mesh on various metal nanoparticles, and also influence of additives, such as sulfur or oxygen, on the graphitization ability of transition metals via semi-empirical molecular orbital calculations. [1] Y. Shibuta, J.A. Elliott, Chem. Phys. Lett., 427, 365-370 (2006). [2] Y. Shibuta and S. Maruyama, Comp. Mater. Sci., 39, 842-848 (2007).

**K1.00340** Investigation of a potential force-generation machinery driven by a cytoskeletal Walker-type ATPase in prokaryotic cells, ANDREAS ERBE, SING-YI HOU, CHEN-YUN CHEN, YI-LIH LIN, JIE-PAN SHEN, LI-JING LIN, CHIA-FU CHOU, YU-LING SHIH, Academia Sinica — Cytoskeletal proteins are often involved in generating mechanical force to drive various cellular processes. A subgroup of the Walker-type ATPases acts as cytoskeletal proteins that show highly dynamic behavior in bacterial cells. One of the most prominent examples is MinD that works with other cellular components to prevent cell division at unwanted polar sites through cycles of pole-to-pole oscillation in E. coli cells. We use fluorescence microscopy techniques to study the process of MinD assembly and disassembly on a lipid bilayer membrane surface and any possible change of membrane properties caused by MinD association with the membrane. To form a supported bilayer membrane, vesicles of the polar or total extract of E. coli membrane or synthetic lipids of defined composition are adsorbed to a treated glass coverslip. Ca\(^{2+}\) is added to enable vesicle fusion to form a continuous bilayer on a glass surface. Formation of a bilayer is examined using fluorescence recovery after photobleaching. The results on the protein assembly on membranes present an important step in understanding the intermediate stages that occur during the dynamic movement of MinD in cells.

**K1.00341** Resistive Small-World Networks, ALICE KOLAKOWSKA, Florida Institute of Technology — The focus of this study is small-world network where there are at least two network paths between any two nodes and the edges have uniform Ohmic resistance. Assuming that signals can locally propagate along the edges between nearest-neighbor nodes due to only potential difference between the nodes, the question being asked is about the global propagation of signals through the network. Simulations demonstrate that the average equivalent resistance of random conductive network follows the average geodesic path but only for highly-connected networks. One physical realization of this situation are conduction paths observed during electrical breakdown.
Tuesday, March 11, 2008 2:30PM - 5:30PM –
Session L1 APS DAMOP: Nobel Prize Session followed by Onsager Prize Session Morial Convention Center LaLouisiane AB

2:30PM L1.00001 Recent developments and perspective in spintronics, A. FERT, UMR CNRS/Thales, 91767 Palaiseau and Université Paris-Sud, 91405 Orsay, France — Recent developments and perspective in spintronics: A. Fert, UMR CNRS/Thales, 91767 Palaiseau and Université Paris-Sud, 91405 Orsay, France After an introduction on the fundamentals of spin transport and the discovery of GMR, I will focus on the most recent developments in spintronics. I will first describe the field of the spin transfer phenomena by reviewing experimental results on magnetic switching and generation of microwave oscillations by spin transfer. The synchronization and phase locking of a collection of STOs (Spin Transfer Oscillators) is an example of new important problem raised by the experiments of spin transfer. I will present data on the synchronization of electrically connected STO. I will then continue the review with results on spintronics with semiconductors, molecular spintronics and spin Hall effect.

Acknowledgements: I thank all the coworkers of my recent works on spintronics, A. Anane[1], J. Barnas [2], A. Barthlmy [1], A. Bernand-Mantel [1], M. Bibes [1], O. Boulle [1], V. Cros [1], C. Deranlot [1], M. Elsen [1], G. Faini [3], B. Georges [1], J. M. George [1], R. Giraud [3], M. Gmitra [2], J. Grollier [1], A. Hamzic [5], L. Hueso [6], H. Jaffrs [1], S. Laribi [1], A. Lemaitre [3], P. M. Levy [7], N. Mathur [6], R. Mattana [1], F. Petroff [1], P. Seneor [1], F. Van Dau [1], A. Vauras [1].

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3:06PM L1.00002 From spinwaves to Giant Magnetoresistance (GMR) and beyond, PETER GRUENBERG1. Institut fuer Festkoerperforschung Forschungszentrum Juelich — Standing spinwaves and surface waves in layered magnetic structures can be used for the detection and quantitative evaluation of interlayer exchange coupling (IEC). Using this method antiferromagnetic IEC has been found in Fe/Cr/Fe layered structures. This was applied to switch the alignment of the magnetizations of the Fe films in an external field from antiparallel to parallel whereby the Giant Magnetoresistance (GMR) effect was discovered. Currently the interest focuses on “Current Induced Magnetic Switching” (CIMS) which can be understood as inverse GMR effect. For all three effects, IEC, GMR and CIMS there are many interesting applications.

1Presented as Nobel lecture in Stockholm on 8th December, 2007

3:42PM L1.00003 Lars Onsager Prize Talk: Quantum fluids: from liquid helium to cold atoms, CHRISTOPHER PETHICK, Nordita and University of Copenhagen — The study of quantum liquids has led to ideas and concepts of broad applicability. I shall illustrate this by examples from the physics of liquid helium-3, heavy-fermion compounds, quark-gluon plasmas and cold atomic gases.

4:18PM L1.00004 Lars Onsager Prize Talk: Stepping through forty years of quantum fluids, GORDON BAYM, University of Illinois at Urbana-Champaign — This talk will trace milestones in quantum fluids from dilute solutions of He-3 in He-4, to superfluids in neutron stars, to cold atoms.

4:54PM L1.00005 Lars Onsager Prize Talk: A New Challenge for Cold Atom Physics: Achieving the Strongly Correlated Regimes for Cold Atoms in Optical Lattices, TIN-LUN (JASON) HO, The Ohio State University — Cold atoms in optical lattices show great promise to generate a whole host of new strongly correlated states and to emulate many theoretical models for strongly interacting electronic systems. However, to reach these strongly correlated regimes, we need to reach unprecedented low temperatures within current experimental settings. To achieve this, it is necessary to remove considerable amount of entropy from the system. Here, we point out a general principle for removing entropies of quantum gases in optical lattices which will allow one to reach some extraordinarily low temperature scales.

3Work supported by NSF Grant DMR0750989 and by DARPA under the Army Research Office Grant No. W911NF-07-1-0464

Tuesday, March 11, 2008 2:30PM - 4:54PM –
Session L2 DCMP DMP: The Physics of Next Generation Photovoltaics Morial Convention Center LaLouisiane C

2:30PM L2.00001 Nano-Structured Silicon Thin Films for Photovoltaic Applications, P. CRAIG TAYLOR, Colorado School of Mines — The current technology for thin-film silicon photovoltaic panels is based on hydrogenated amorphous silicon and related alloys, such as silicon-germanium and silicon-carbon. Currently there is great interest in using some form of thin-film silicon that includes nano-structured components. This interest is driven in part by the potential for decreased cost, increased efficiency, and increased stability. Also driving this interest is the abundance of silicon as an element and its lack of toxicity. I will review various structures that have been suggested, and discuss recent results on inhomogeneous films of hydrogenated amorphous silicon that contain nanocrystalline inclusions. In particular, I will describe the mechanisms for optical absorption, carrier transport and the role of defects.
mechanisms at electrochemical interfaces; an efficiency and reliability with industrial credibility have been demonstrated and verified, and a significant role in production. G24 Innovations PLC in Wales is commissioning a manufacturing plant, and Dyesol PLC in Australia is making available the required materials certified, and a stability of over 14,000 hours under accelerated testing with continuous simulated AM1.5 illumination was recently reported. In consequence and frequently a nanodispersed Pt precipitated from hexachloride solution is employed. It is by now evident that the achievement of an industrially-competitive dye—semiconductor bond. A wide range of organic systems were therefore investigated, with the present favored formulation being based on imidazole salts. The iodine/iodide system, with the advantage that the ions, both oxidized and reduced are relatively small, and therefore mobile in the supporting electrolyte. Energy therefore a sophisticated molecular engineering product. The electrolyte is also an optimized electrochemical system. The basic redox behavior is provided by the modified by substitution with thiocyanide groups. Chemisorptive attachment of the dye to the metal oxide surface is obtained by carboxyl groups attached properties expected. A ruthenium-pyridyl complex provides the chromophore of the dye, with the HOMO-LUMO gap, and thence the absorption spectrum bring convenient thin-film process such as screen printing or tape casting. The preferred dye system is inspired by the natural processes involving chlorophyll, the can be determined by hydrothermal processing of a precursor sol, and the film can be deposited on a transparent conducting oxide (TCO) substrate by any photoelectrochemical applications is titanium dioxide in the anatase crystal structure. The size of the nanocrystals making up the semiconductor photoanode also a highly-disordered, even porous, semiconductor structure is acceptable, enabling surface adsorption of a sufficient concentration of the dye to permit total absorption of incident light of photon energy greater than the HOMO-LUMO gap of the dye molecule. The accepted wide-band semiconductor for photovoltaic applications is titanium dioxide in the anatase crystal structure. The size of the nanocrystals making up the semiconductor photoanode can be determined by hydrothermal processing of a precursor sol, and the film can be deposited on a transparent conducting oxide (TCO) substrate by any convenient thin-film process such as screen printing or tape casting. The preferred dye system is inspired by the natural processes involving chlorophyll, the coloring material in plants on which all earthly life depends. Chlorophyll is an organometallic dye, with a metal ion, Mg, within a porphyrin cage of nitrogen atoms. The synthetic chemist of course can select any convenient metal within the periodic table, and experience shows that ruthenium has the optimal properties expected. A ruthenium-pyridyl complex provides the chromophore of the dye, with the HOMO-LUMO gap, and thence the absorption spectrum bring modified by substitution with thiocyanide groups. Chemisorptive attachment of the dye to the metal oxide surface is obtained by carboxyl groups attached to the pyridyl components. The energetics of the dye is that the LUMO level is just above the conduction band edge of the semiconductor, enabling relaxation by electron injection as required. A satisfactory electroactive dye structure, with good attachment properties and a wide optical absorption spectrum is therefore a sophisticated molecular engineering product. The electrolyte is also an optimized electrochemical system. The basic redox behavior is provided by the iodine/iodide system, with the advantage that the ions, both oxidized and reduced are relatively small, and therefore mobile in the supporting electrolyte. Energy losses due to slow diffusion is minimized. Early experiments used aqueous electrolytes, though with limited cell lifetime due to hydrolysis of the chemisorptive dye—semiconductor bond. A wide range of organic systems were therefore investigated, with the present favored formulation being based on imidazole salts. These have the additional advantage of low vapour pressure, thereby avoiding as a photovoltaic system the mid—day sun illumination may reach 80 °C or higher. Low losses at the cathode counter electrode are also a requirement for cell efficiency. The cathode is not necessarily transparent, and prototype cells on thin metal foils have been produced. However a TCO on glass or polymer counter electrode is widely used. In either case suitable electrolytically behavior is required and frequently a nanodispersed Pt precipitated from hexachloride solution is employed. It is by now evident that the achievement of an industrially-competitive sensitized photoelectrochemical solar cell is the result of the optimization of several components, associated obviously with their effective synergy. Each change of a single component has repercussions on the choice and performance of others. However as already mentioned an efficiency of over 11% has now been certified, and a stability of over 14,000 hours under accelerated testing of continuous simulated AM1.5 illumination was recently reported. In consequence there is increasing confidence on the part of industry. Several licensees of EPFL patents on dye—sensitized photo voltaic cells are now preparing for large-scale production. Dyesol PLC in Wales is commissioning a manufacturing plant, and Dyesol PLC in Australia is making available the required materials on an industrial scale. In conclusion, then, it can be stated that the DSC system is much more than a fascinating scientific artifact illustrating charge-transfer mechanisms at electrochemical interfaces; an efficiency and reliability with industrial credibility have been demonstrated and verified, and a significant role in competition with other photosystems can be foreseen.
2:30PM L3.00001 The Disordered Kinetics of Earth’s Carbon Cycle

Discussed at a simple box model of soil-vegetation-atmosphere interactions that we recently introduced to study the insulation of summer droughts at continental midlatitudes (D’Andrea et al, GRL 2006, Baudena et al, AWR 2007). I show that the model possesses multiple equilibria and that, for the same synoptic forcing, soil moisture at the beginning of summer and vegetation cover play a primary role in determining which equilibrium will be reached. We also observe a difference in the drought climatologies associated especially with the dynamics of natural vegetation, capable of adapting to the prevailing soil moisture conditions, and with cultivated vegetation such as eggplant, that cannot spontaneously modify its areal extent. I conclude with some speculations on a conceptual model of the interaction between vegetation and climate at global scale. The results discussed in this talk are the product of joint work with Fabio D’Andrea (ENS, Paris) and Mara Baudena (ISAC-CNR).

3:06PM L3.00002 The Quantum and Fluid Mechanics of Global Warming

Support in part by NSF grant no. DMR-0605619.


3:42PM L3.00003 Geostrophic Turbulence and the stability of Ocean models

ANNALISA BRACCO, Georgia Tech — Despite multiple efforts, predictions of climate change remain uncertain. Where precision is an issue (e.g., in a climate forecast), only ensembles of simulations made across model families which differ for parameterizations, discrete algorithms and parameter choices allow an estimate of the level of uncertainty. Is this the best we can do? Or is it at least conceptually possible to reduce these uncertainties? Focusing on ocean models in idealized domains we describe chaotic space-time patterns and equilibrium distributions that mimic nature. Using the Navier-Stokes equations for barotropic flows as a zero-order approximation of analogous flow pattern, we then investigate if it is possible, in this overly-simplified set-up, for which smooth-solutions exist, to bound the uncertainty associated with the numerical domain discretization (i.e. with the limitation imposed by the Reynolds number range we can explore). To do so we analyze a series of stationary barotropic turbulence simulations spanning a range of Reynolds number of 10^3.

4:18PM L3.00004 Heat waves, climate change and eggplant harvests - simple models of climate systems

ANTONELLO PROVENZALE, ISAC-CNR, Torino, Italy — I discuss a simple box model of soil-vegetation-atmosphere interactions that we recently introduced to study the insulation of summer droughts at continental midlatitudes (D’Andrea et al, GRL 2006, Baudena et al, AWR 2007). I show that the model possesses multiple equilibria and that, for the same synoptic forcing, soil moisture at the beginning of summer and vegetation cover play a primary role in determining which equilibrium will be reached. We also observe a difference in the drought climatologies associated especially with the dynamics of natural vegetation, capable of adapting to the prevailing soil moisture conditions, and with cultivated vegetation such as eggplant, that cannot spontaneously modify its areal extent. I conclude with some speculations on a conceptual model of the interaction between vegetation and climate at global scale. The results discussed in this talk are the product of joint work with Fabio D’Andrea (ENS, Paris) and Mara Baudena (ISAC-CNR).

4:54PM L3.00005 Physical Problems in Modeling the Global Ocean

STEPHEN GRIFFIES, NOAA/Geophysical Fluid Dynamics Lab — Understanding and modeling the physical ocean circulation is of primary importance for both enhancing the science of the ocean, and for providing rational projections of future climate. This talk aims to outline fundamental physical and numerical aspects of ocean climate modeling. We highlight features associated with representing elements of the continuum ocean fluid using a discrete model lattice. A major challenge of this representation includes the parameterization of scales which are unresolved by the simulation. This subgrid-scale problem is ubiquitous in computational fluid dynamics, and forms a major focus of ongoing research and development with ocean climate models. Another challenge involves developing robust numerical methods whose truncation errors do not adversely corrupt the quasi-ideal nature of much of the ocean circulation outside of boundary layers. Progress has been made on both fronts, with improvements arising from better understanding of the ocean, smarter methods used to simulate the ocean, and enhancements in computational power.

Tuesday, March 11, 2008 2:30PM - 4:54PM Session L4 DCMP: Bosonic Modes in HTSC

2:30PM L4.00001 STM Observation of a Bosonic Mode in the Electron-Doped Superconductor

2\text{0}_{0.88}\text{LaCe}_{0.12}\text{CuO}_{4-\delta} \text{, VIDYA MADHAVAN, Boston College — Information on bosonic excitations in high temperature superconductors is part of a critical dataset that is necessary to decipher the physics of the pairing mechanism in these materials. In this talk, I will discuss our recent STM investigations of the electron-doped cuprate superconductor 2\text{0}_{0.88}\text{LaCe}_{0.12}\text{CuO}_{4-\delta} (PLCCO) (T_c = 24 K). Our spectra reveal superconducting gaps with coherence peaks that disappear above T_c. In addition, multiple step/peak-like features are observed outside the gap. Such features in STM spectra are suggestive of bosonic excitations that couple strongly to the electrons. Analysis of the data indicates that the observed (bosonic) mode energy in PLCCO lies at 10.5 \pm 2.5 meV which is much lower than the bosonic mode observed in hole-doped BSCCO. The energy scale of our mode is the same as the magnetic resonance mode (spin-excitations) in PLCCO measured by inelastic neutron scattering but is also consistent with a low energy acoustic mode. Additionally, I will show that both the local mode energy and the intensity reveal correlations with the local gap energy scale. The sensitivity of the mode intensity to the energy scale of the onset of the continuum of excitations (\Delta) may indicate an electronic origin rather than phonons. This work was done in collaboration with F. C. Nietsenski, S. Kunwar, S. Zhou, Shiliang Li, H. Ding, Ziqiang Wang, and Pengcheng Dai.
3:06PM L4.00002 Bosonic self energy spectrum of high temperature superconductors from optical spectroscopy1. THOMAS TIMUSK, McMaster University — We address the problem of extracting the bosonic spectral function in high temperature superconductors using optical spectroscopy. Last year, we succeeded in inverting the optical spectra of the cuprates and extract the quantity, analogous to the electron-phonon spectral density $\alpha^2 F(\omega)$ in the conventional superconductors, for YBCO Ortho II system. We used the highly ordered crystals grown by Hardy, Bonn and Liang and compared our results with magnetic neutron spectra on samples from the same source measured by Stock et al. There was excellent agreement between the results of the two sets of spectroscopies. Since then we have refined our inversion technique and have been able to make a similar comparison for the LSCO system with new neutron scattering data from Vignolle et al. This magnetic spectrum, together with our Eliashberg inversion, accounts in a straightforward way for the lower $T_c$ of LSCO as compared to other cuprates. We also offer a detailed prediction of the evolution of the magnetic excitation spectrum with temperature and doping for the highly studied system Bi-2212, a material were neutron scattering data are very hard to get. Our data show that the bosonic self energy function evolves continuously from the broad background.

1Work done in collaboration with Jungseok Hwang, Jules Carbotte and Ewald Schachinger

3:42PM L4.00003 Visualizing pair formation in $Bi_2Sr_2CaCu_2O_{x=2.5}$. ABHAY PASUPATHY, Princeton University Physics Dept. — Unlike traditional superconductors, the density of states (DOS) of the high-Tc superconductor $Bi_2Sr_2CaCu_2O_{x=2.5}$ shows large nanoscale variations that have been detected using scanning tunneling microscopy (STM) [1,2]. Such variations are seen in the low temperature superconducting gap [1] and in features associated with the coupling of pairs to boson modes [2]. In order to understand these variations in the spectra, we perform atomic resolution STM measurements of $Bi_2Sr_2CaCu_2O_{x=2.5}$ as a function of temperature [3]. Using newly developed experimental techniques, we measure the evolution of the DOS from low temperature ($T<<Tc$) to temperatures where all gaps in the spectrum have disappeared ($T>T^*$). Such measurements show that the pairing gap nucleates in nanoscale regions at temperatures between $Tc$ and $T^*$. By normalizing the low temperature DOS ($T<<(Tc)$ to the DOS at high temperature, we are able to fit the superconducting DOS to the d-wave BCS form. We find that the experimental spectrum deviates from a simple d-wave fit indicating a strong coupling between electrons and bosonic modes. We will discuss the temperature evolution of these as well as other features in the DOS, and correlate such measurements with the inhomogeneity seen in the gap magnitude at low temperature.


Work in collaboration with Kenjiro Gomes, Aakash Pushp, Colin Parker, Shimpei Ono, Genda Gu, Yoichi Ando and Ali Yazdani.

3:48PM L4.00004 Evolution of the gaps through the cuprate phase-diagram. ALAIN SACUTO, University Denis Diderot- Paris 7 — The actual physical origin of the gap at the antinodes, and a clear identification of the superconducting gap are fundamental open issues in the physics of high-Tc superconductors. Here, we present an electronic Raman scattering study of single layer cuprates, as a function of both doping level and temperature. We examine both the evolution of the gaps close to the nodes and at the antinodes in the normal and superconducting sates. On the deeply over-doped side, we show that the anti-nodal gap is a true superconducting gap. In contrast, on the under-doped side, our results reveal the existence of a break point close to optimal doping below which the anti-nodal gap is gradually disconnected from superconductivity. The nature of both the superconducting and normal state is distinctly different on each side of this break point and will be discussed.


Tuesday, March 11, 2008 2:30PM - 5:30PM – Session L5 DCMP: Phase Transitions in Disordered Magnets

2:30PM L5.00001 Dilute anisotropic dipolar systems as random field Ising ferromagnets, MOSHE SCHECHTER, University of British Columbia — We have shown the equivalence, at low energies, of dilute anisotropic dipolar magnets to the Ising model in the presence of an effective randomly longitudional field and an effective transverse field, both of which are independently tunable. In the ferromagnetic (FM) regime, these systems constitute the first realization of the classical, as well as quantum, random field Ising model in a FM system, allowing, in particular, the application of a longitudinal field conjugate to the FM order parameter. In the spin-glass regime [2,3] we elucidate the role of both the hyperfine interactions, which couple the system to a spin bath and change the low-energy degrees of freedom, and the off-diagonal terms of the dipolar interactions, which lead to the effective random field. This resolves long standing questions regarding quantum spin glasses in general, and the quantum phase transition between the spin glass and paramagnetic phases in particular.

1. LiHo$_2$Y$_{1-x}$F$_3$ as a random field Ising ferromagnet, M. Schechter, Cond-mat/0611063.

3:06PM L5.00002 A ferromagnet in a continuously tuneable random field1. D.M. SILEVITCH, James Franck Institute/University of Chicago — The Random-Field Ising Model (RFIM) has been extensively studied as a model system for understanding the effects of disorder in magnets. Since the late 1970s, there has been a particular focus on realizations of the RFIM in site-diluted antiferromagnets. We observe random-field effects in the dilute dipole-coupled ferromagnet LiHo$_2$Y$_{1-x}$F$_3$. In the presence of a magnetic field transverse to the Ising axis ($H_z$), the behavior of LiHo$_2$Y$_{1-x}$F$_3$ becomes increasingly dominated by the influence of random-field terms in the effective Hamiltonian. This is seen experimentally in the shape of the ferromagnetic-paramagnetic phase boundary and in changes to the critical exponents near the classical critical point. We find that above the classical critical point the magnetic susceptibility diverges as $H_z \to 0$, and that the susceptibility both above and below the classical critical point can be collapsed onto a single universal curve using a modified Curie law which explicitly incorporates random-field contributions. The discovery of a ferromagnetic realization of the RFIM opens the door to investigation of the random-field problem with the wide variety of techniques available for probing ferromagnets, including the ability to examine both the statics and dynamics of the random-field problem. It also allows studying the effects of controlled amounts of randomness on the dynamics of domain pinning and the energetics of domain reversal.

1Performed in collaboration with D. Bitko, J. Brooke, S. Ghosh, G. Aeppli, and T.F. Rosenbaum. The work in Chicago was supported by NSF and DOE BES, while work in London was supported by the UK EPSRC and a Wolfson-Royal Society Research Merit Award.
3:42PM L5.00003 Activated quantum criticality of complex systems, BERNARD BARBARA, CNRS, Institut Néel, Grenoble — Magnetization measurements performed on single crystals of Ho$_{x}$Y$_{1-x}$LiF$_4$ with $x \approx 16.5\%$ and 4.5\% show the same behavior for both compositions: (i) absence of divergence of the non-linear susceptibility in a transverse field (ii) same absence of divergence in zero field. These results are in sharp contrast with earlier studies of Ho$_{x}$Y$_{1-x}$LiF$_4$. In (i) the observed lack divergence results from the presence of random fields induced by the applied transverse field (no spin-glass phase transition, as predicted by Schechter, Laflorencie and Stamp). In (ii) its results from important slowing down of the dynamics due to huge energy barriers. Excellent fits for the linear and non-linear susceptibilities with $\ln(M) = -T / (H, T)$ ($\Gamma$ is a functional form), suggesting the possibility of a dynamical phase transition involving thermally activated tunneling states. This model may also be useful for more general quantum dynamics of complex systems at finite temperatures. Scaling of non-linear susceptibility in MnCu and GdAl spin-glasses, Barbara, A. P. Malozemoff, and Y. Imry, PRL, 7, 1852 (1981).


Nuclear spin driven quantum relaxation in LiHo$_{0.002}$Y$_{0.998}$F$_{4}$, R. Giraud, W. Wernsdorfer, A. M. Tkachuk, D. Mailly, and B. Barbara, PRL, 87, 057203 (2001).

Significance of the hyperfine interactions in the phase diagram of LiHo$_{x}$Y$_{1-x}$F$_4$, M. Schechter and P. C.E. Stamp, PRL, 95, 267208 (2005).


3:42PM L6.00003 Use of X-ray absorption spectroscopy in the search for the best LIGO mirror coatings1. STEPHEN C. MCGUIRE, Southern University and A&M College — The Laser Interferometer Gravitational-wave Observatory (LIGO) seeks to improve its sensitivity for gravity-wave detection by a factor of ten during the next phase of operation. Advanced LIGO. In order to achieve this goal it is necessary to design and fabricate test mass mirrors that help minimize the noise in the interferometers and in doing so maximize gravity-wave detection capability. In this talk we will present recent results from our program of X-ray absorption spectroscopy measurements to obtain detailed chemical composition and structure of titania (TiO2)-doped tantala (Ta2O5) multilayers fabricated via ion beam sputtering on SiO2 substrates. Our investigations focus on how the microscopic features of the coatings influence their macroscopic mechanical loss properties. Our goal is to obtain correlations between chemical imurities and/or dopants and the optical and mechanical loss characteristics of these multilayer coatings. To examine our samples we use synchrotron-based X-ray absorption Spectroscopy (XAS) techniques including Extended X-ray Absorption Fine Structure (EXAFS), X-ray Absorption Near Edge Structure (XANES) and X-ray Fluorescence (XRF). We present chemical and structural data obtained at the titanium K-edge and tantalum L2,3-edge as well as relative elemental distribution information (Ti/Ta, Fe/Ta, and Cr/Ta) obtained via XRF. Following a brief description of the LIGO experiment, our program of research in optical materials for use in advanced versions of the interferometer will be described.

1Work supported by National Science Foundation Grants No(s). PHY-0101177 and PHY-0701652.

4:18PM L6.00004 A Mathematical Solution to the Theoretical Band Gap Underestimation: Predictive Calculations of Properties of Semiconductors1. DIOLA BAGAYOKO, Southern University and A&M College — Most density functional theory (DFT) calculations find band gaps that are 30-50 percent smaller than the experimental ones, as illustrated in this presentation that recalls some popular explanations of this band gap problem, i.e., self-interaction effects and derivative discontinuities of the exchange correlation energy. A survey of the increasingly numerous approaches aimed at resolving the theoretical underestimation follows these explanations. These approaches include the Green function and screened Coulomb approximation (GWA), time dependent density functional theory (TDDFT), the exact exchange and screened exchange methods, and the use of local density approximation (LDA) potentials plus additional potentials located at atomic sites. Using the Rayleigh theorem, we describe a basis set and variational effect inherently associated with calculations that employ a linear combination of atomic orbitals (LCAO) in a variational approach of the Rayleigh-Ritz type. This description concomitantly shows a source of large underestimation errors in calculated band gaps, i.e., an often dramatic lowering of some unoccupied energies on account of the Rayleigh theorem as opposed to the Hamiltonian. We present the Bagayoko, Zhao, and Williams (BZW) method [Phys. Rev. B 60, 1563 (1999); PRB 74, 245214 (2006); and PRB 76, 037101 (2007)] that follows from the description of the aforementioned effect and that leads (a) to DFT and LDA calculated band gaps of semiconductors in agreement with experiment and (b) theoretical predictions of band gaps that are confirmed by experiment. Unlike most calculations, BZW computations solve, self-consistently, a system of two coupled equations. DFT-BZW calculated mass and optical properties (dielectric functions) also agree with measurements. We illustrate ten years of success of the BZW method with its results for GaN, C, Si, 3C-SiC, 4H-SiC, ZnO, AlN, CaF2, ZnSe, w-InN, InAs, and AlN. We conclude with a request to revisit beliefs relative to actual limitations of DFT and of schemes purporting to correct it or to go beyond it.

1Work funded in part by the Department of the Navy, Office of Naval Research (ONR, Award Nos. N00014-05-1-0830 and N00014-05-1-0009), NASA (NNG 05G146G), and the National Science Foundation (NSF, Award No. HRD 0503362).

4:54PM L6.00005 New Possibilities for Understanding Complex Metal Hydrides via Synchrotron X-ray Studies1. TABETHA DOBBINS, Grambling State University and Louisiana Tech University — Ultrasmall-angle x-ray scattering (USAXS) and X-ray absorption spectroscopy (XAS) are used for the study of chemical and morphological changes in metal hydride powder (e.g. NaAlH4) both before and after transition metal salt catalytic dopant additions by high energy ball milling. The variation in surface fractal dimension and particle size with milling time and dopant content were tracked. These studies show that dopant content level (e.g. 2 mol % and 4 mol %) and dopant type (i.e. TiCl2, TiCl3, VC3, and ZrCl4) markedly affects NaAlH4 powder particle surface area (determined using USAXS surface fractal dimension). As well, the chemical reaction between the catalyst and hydride powder was further elucidated using XAS. Ti-metal reacts with the Al desorption product (NaAlH4) to form TiAlx product phases. These studies were able to link powder particle surface area to catalytic doping and were able to link dopant chemical state with dehydrogenation reactant and product phases.

1Support from the Dept. of Energy, Basic Energy Sciences and the National Science Foundation, Division of Materials Research is gratefully acknowledged.

Tuesday, March 11, 2008 2:30PM - 5:30PM –
Session L7 DBP GSNP: Multiscale Phenomena in Biological Physics Morial Convention Center R05

2:30PM L7.00001 Self assembly of natural and synthetic membranes using coarse grain models , MICHAEL L. KLEIN, University of Pennsylvania — The talk will review recent work by the Klein group in deriving force fields for natural and synthetic membrane forming systems. Molecular dynamics studies of the self-assembly will be presented for both types of systems.

3:06PM L7.00002 Bridging time-scale gaps via reaction path optimization , JHIH-WEI CHU, Department of Chemical Engineering, University of California, Berkeley — In this talk I will present a series of new computational methodologies that can be applied to systematically investigate the mechanism, free energy profiles, and rates of large-scale conformational changes of biomolecules. First, we enhance the efficiency of reaction path optimization methods, which use a series of duplicated systems, or replicas, to represent a discrete path by using holonomic constraints instead of reparametrization or using penalty potential functions that measure its next phase of operation. Advanced LIGO. In order to achieve this goal it is necessary to design and fabricate test mass mirrors that help minimize the noise in the interferometers and in doing so maximize gravity-wave detection capability. In this talk we will present recent results from our program of X-ray absorption spectroscopy measurements to obtain detailed chemical composition and structure of titania (TiO2)-doped tantala (Ta2O5) multilayers fabricated via ion beam sputtering on SiO2 substrates. Our investigations focus on how the microscopic features of the coatings influence their macroscopic mechanical loss properties. Our goal is to obtain correlations between chemical imurities and/or dopants and the optical and mechanical loss characteristics of these multilayer coatings. To examine our samples we use synchrotron-based X-ray absorption Spectroscopy (XAS) techniques including Extended X-ray Absorption Fine Structure (EXAFS), X-ray Absorption Near Edge Structure (XANES) and X-ray Fluorescence (XRF). We present chemical and structural data obtained at the titanium K-edge and tantalum L2,3-edge as well as relative elemental distribution information (Ti/Ta, Fe/Ta, and Cr/Ta) obtained via XRF. Following a brief description of the LIGO experiment, our program of research in optical materials for use in advanced versions of the interferometer will be described.

3:42PM L7.00003 A Novel Empirical Potential Function and A Monte Carlo Sampling Technique , JIANPENG MA, Baylor College of Medicine — In protein folding study, two major issues are effective potential function and powerful sampling technique. In this meeting, recent results in both directions will be presented. In terms of potential function, we have developed an orientation-dependent statistical all-atom potential derived from side-chain packing. Test of the new potential on decoy set recognition indicates that it outperforms all the known statistical potential functions in the literature. Applications of this potential in substantially improving side-chain modeling will also be discussed. In terms of sampling technique, I will discuss some new results of a novel Monte Carlo sampling technique that performs simulation via direct computation of partition functions. The results will be compared with those of the well-known Wang-Landau sampling scheme. Application of this new MC method in studying protein folding will also be discussed.

1Work supported by National Science Foundation Grants No(s). PHY-0101177 and PHY-0701652.
J. C. Crocker and D. G. Grier, analyzed. The interaction between two isolated droplets was calculated from their trajectories through the Markovian dynamics extrapolation method developed. The dynamics of droplets at interface were imaged using optical microscopy, from which the droplets' motions were tracked and droplets eliminated surface roughness and thus reduced the complexity of the system. We captured micron-sized oil droplets at water-air interface and measured attraction, but the possibility remains that attraction arises from an irregular contact line on the particles' surfaces. Replacing the solid particles with liquid 1 long-range attraction among microparticles at fluid interfaces. Recent theoretical work represents the simplest system which can capture one of the relevant components of multi-body interactions, the fact that while two particles can freely rotate anisotropy of MOON (Modulated Optical Nanoprobes) particles to simultaneously measure their translation and rotation in an optical microscope. This system — Three colloidal particles were placed in small corrals and the strong correlations between their translation and rotation were quantified using the optical — A large variety of nanoparticles holds extraordinary promises for practical applications, e.g., in catalysis and materials science. For these and other applications it is necessary to assemble the nanoparticles to yield supra-molecular aggregates of desired morphology. We are interested in the self-assembly of spherical colloids (i.e., nanoparticles) induced by interactions that become anisotropic because of entropic effects. Thus short polymer brushes are grafted on restricted regions of the spherical nanoparticles considered (e.g., the equatorial plane). Monte Carlo simulations were conducted to assess the properties of the self-assembled nanostructures as a function of the length of the brushes and of the strength of the particle-particle attraction. Depending on the specific solution conditions (particle-particle dispersive attractions, as well as length and density of the grafted polymer brushes) it is possible to obtain uniform dispersions, irregular aggregates, spherulites, one-dimensional wires, and two-dimensional colloidal sheets. We will discuss whether or not the effective colloid-colloid pair interactions at infinite-dilute conditions (i.e., the potential of mean force) can be used to predict the emerging behavior of the colloidal nanoparticles at larger concentrations.

2:42PM L9.00002 Emerging Structures for Colloidal Brushes: from Dispersions and Agglomerates to Spherulites, Wires, and beyond. ALBERTO STRIOLO, University of Oklahoma — A large variety of nanoparticles holds extraordinary promises for practical applications, e.g., in catalysis and materials science. For these and other applications it is necessary to assemble the nanoparticles to yield supra-molecular aggregates of desired morphology. We are interested in the self-assembly of spherical colloids (i.e., nanoparticles) induced by interactions that become anisotropic because of entropic effects. Thus short polymer brushes are grafted on restricted regions of the spherical nanoparticles considered (e.g., the equatorial plane). Monte Carlo simulations were conducted to assess the properties of the self-assembled nanostructures as a function of the length of the brushes and of the strength of the particle-particle attraction. Depending on the specific solution conditions (particle-particle dispersive attractions, as well as length and density of the grafted polymer brushes) it is possible to obtain uniform dispersions, irregular aggregates, spherulites, one-dimensional wires, and two-dimensional colloidal sheets. We will discuss whether or not the effective colloid-colloid pair interactions at infinite-dilute conditions (i.e., the potential of mean force) can be used to predict the emerging behavior of the colloidal nanoparticles at larger concentrations.

2:54PM L9.00003 Roughness-controlled depletion interactions for controlling colloidal self-assembly. KUN ZHAO, Dept. of Chemistry, University of California- Los Angeles, THOMAS G. MASON, Deps. of Physics and Chemistry, University of California- Los Angeles — The surfaces of colloidal particles resulting from many new fabrication methods are not molecularly smooth, so understanding how the surface roughness affects the depletion attraction is very important. We show that the depletion attraction between custom-shaped microscale platelets can be suppressed when the nanoscale surface asperity heights become larger than the depletion agent. In the opposite limit, the attraction re-appears and columnar stacks of platelets are formed. Exploiting this, we selectively increase the site-specific roughness on only one side of the platelets to direct the mass-production of a single desired assembly, a pure dimer phase. Furthermore, we model the interaction between flat plates coated by hemispheres having controlled sizes and densities relative to those of a spherical depletion agent. Overall, these studies provide significant insight into attractive bonds between particles that retain lubrication, and they provide a basis through which more complex assemblies can be made.

3:06PM L9.00004 Corralled Colloids in Four Dimensions. STEPHEN ANTHONY, Department of Chemistry, University of Illinois, MINSU KIM, Department of Physics, University of Illinois, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois — Three colloidal particles were placed in small corrals and the strong correlations between their translation and rotation were quantified using the optical anisotropy of MOON (Modulated Optical Nanoprobes) particles to simultaneously measure their translation and rotation in an optical microscope. This system represents the simplest system which can capture one of the relevant components of multi-body interactions, the fact that while two particles can freely rotate together (like gears), once a third particle (or gear) is added there is no universally favorable set of rotations. This single multi-body system provides a paradigm of how rotation influences translation and vice-versa.

3:18PM L9.00005 Interactions among microdroplets at the water-air interface. CHUAN ZENG, Department of Physics, University of Massachusetts Amherst, ANTHONY D. DINSMORE — There has been a great mystery concerning the origin of measured long-range attraction among microparticles at fluid interfaces. Recent theoretical work showed that electrostatic interactions should not lead to long-range attraction, but the possibility remains that attraction arises from an irregular contact line on the particles' surfaces. Replacing the solid particles with liquid droplets eliminated surface roughness and thus reduced the complexity of the system. We captured micron-sized oil droplets at water-air interface and measured the interaction between them. The dynamics of droplets at interface were imaged using optical microscopy, from which the droplets' motions were tracked and analyzed. The interaction between two isolated droplets was calculated from their trajectories through the Markovian dynamics extrapolation method developed by J. C. Crocker and D. G. Grier. We acknowledge support from NASA through the Fluid Physics program (NRA 02-OBPR-03-C) and from the NSF-supported MRSEC on Polymers (DME-0213695).


3:30PM L9.00006 Geometrical frustration in colloidal “antiferromagnet”¹, YILONG HAN, Hong Kong University of Science and Technology, YAIR SHOKEF, AHMED ALSAYED, PETER YUNKER, TOM LUBENSKY, ARJUN YODH, University of Pennsylvania — We report experiments about a self-organized colloidal system that exhibits geometrical frustration similar to that of antiferromagnetic Ising spins on a triangular lattice. Novel thermally sensitive microgel NIPA (N-isopropyl acrylamide) spheres are close packed between two parallel flat walls with a vertical separation of about 1.5-particle diameters. The particles form an approximate in-plane triangular lattice. Neighboring particles tend to push each other toward opposite walls leading to out-of-plane local up and down buckling. We tune the strength of such effective antiferromagnetic interactions by varying temperature-tunable diameter of spheres. “Spin” flipping was directly visualized with video microscopy. We investigated the static structures, the dynamics of particles with different degrees of frustration and the degenerated ground state. This experiment is the first dynamic measurement in a geometrical frustrated system at single-particle resolution.

¹This work is supported by the MRSEC grant DMR-0520020 and NSF grant DMR-0505048.

3:42PM L9.00007 Correlated Motion of Ellipsoids Diffusing in 3D, KENNETH DESMOND, ERIC R. WEEKS, Emory University — Currently the hydrodynamic interaction between two ellipsoids in a fluid is not well understood. By observing the Brownian motion of micron sized ellipsoids suspended in a fluid using confocal microscopy, we directly measure these interactions. The ellipsoids exhibit both translational and rotational diffusion. The motion of an ellipsoid induces a flow field, which couples the motion of other ellipsoids with the first one. In our experiments we measure the translational and rotational diffusion of polystyrene ellipsoids suspended in a water glycerol mixture in three dimensions, and examine the spatial correlations between the rotational and translational motion of pairs of ellipsoids. Rotational motions set up a dipolar flow field, and thus the resulting correlations decay quicker than the correlations caused by translations.

3:54PM L9.00008 Simulating Collective Dynamics of Confined Colloids¹, JONATHAN K. WHITMER, ERIK LUITJEN, University of Illinois at Urbana-Champaign — We investigate the dynamical behavior of colloidal particles under confinement, by means of computer simulations that explicitly account for hydrodynamic interactions. Even under dilute conditions, long-range solvent-mediated coupling of the translational and rotational degrees of freedom influences the relative motion of colloidal particles. These effects on the collective dynamics are often ignored in simulations. Our calculations utilize the hybrid Stochastic Rotation Dynamics/Molecular Dynamics method [A. Malevanets and R. Kapral, J. Chem. Phys. 112, 7260 (2000)] to incorporate both hydrodynamic and Brownian forces exerted on colloids by the solvent. The computational results are compared to recent experiments on few-body colloidal systems where the particle number is limited through confinement in a cylindrical trap.

¹This work is supported by the National Science Foundation through Grant No. DMR-0346914.

4:06PM L9.00009 Stripes and their zigzagging in buckled hard spheres, YAIR SHOKEF, University of Pennsylvania, YILONG HAN, Hong Kong University of Science and Technology, AHMED ALSAYED, PETER YUNKER, TOM LUBENSKY, ARJUN YODH, University of Pennsylvania — We use a hard sphere model to describe recent experiments on buckled colloidal monolayers. Our detailed Monte Carlo simulations exhibit the behavior, observed experimentally, of antiferromagnetic order and the formation of stripes that randomly zigzag around the system. Using free volume calculations, we deduce the strength of the effective antiferromagnetic interactions between neighboring particles. We furthermore explain how the geometrical frustration is partially removed by collective effects arising from sphere packing. We show how lattice distortions enable striped configurations to pack better than disordered ground states of the simple antiferromagnetic Ising model and that zigzagging of these stripes does not affect the free volume of the system.

4:18PM L9.00010 Breakdown of Pairwise Additivity in Colloidal Electrostatics¹, SUNIL SAINIS, Yale University, Mechanical Engineering Department, ERIC DUFRESNE, Yale University, Departments of Mechanical Engineering, Chemical Engineering and Physics — Predictions of the structure and stability of charged colloidal suspensions typically assume pairwise additive forces. We directly measure electrostatic forces in small clusters of two to seven particles in a nonpolar solvent. We find that electrostatic interactions are not pairwise additive when the particle separations are much smaller than the screening length.

¹Yale University, Sandia NINE, Cabot Corp.

4:30PM L9.00011 Mystery on Charge Asymmetry: Anionic Macroions in Periodic Lattices Held by Hydrated Cations and Not vice versa¹, WILLIAM KUNG, MONICA OLVERA DE LA CRUZ, Northwestern University — We propose a mean-field analytical model to account for the observed asymmetry in the ability to form long-range attraction by the negatively charged colloidal particles and not their equivalently charged positive counterpart. We conjecture that this asymmetry is due to solvation effects, and we phenomenologically capture its physics by considering the relative strength of this water-induced short-range repulsion between the different charge species. We then apply our model to the colloidal system of negatively charged disks that are neutralized by a sea of counterions and strongly absorbed to an interface in a compressible binary system. We demonstrate the resulting coexistence between a dilute isotropic ionic phase and a condensed hexagonal lattice phase as a function of density and interaction strength.

¹ACS-PCF Grant 44645-AC7.

4:42PM L9.00012 Charged colloids in low polar solvents, ANDREW HOLLINGSWORTH, MIRJAM LEUNISSEN, WILLIAM IRVINE, PAUL CHAIKIN, New York University, ALFONS VAN BLAADEREN, Utrecht University — In a low polar environment, sterically-stabilized poly(methyl methacrylate) spheres become positively charged and exhibit extraordinary long-range repulsive interactions. Confocal microscopy shows that they can form low density, body centered cubic crystals with lattice constants up to 40 microns. We attribute this behavior to the cyclohexyl bromide (CHB) in which the colloidal particles are suspended. CHB is a desirable solvent due to its density matching capability; however, it is difficult to purify. Trace amounts of the hydrogen halide resulting from the hydrolysis of CHB apparently interact with the stabilizer layer, imparting charge to the colloids. Surprisingly, water can also be used to deionize the organic solvent, depending on the relative amounts of the two fluids. The addition of quaternary ammonium salts was used to screen charge (reducing long range particle interaction). Ionic strengths were computed using ionic association theory; in turn, particle charge and surface potentials were estimated from electrokinetic measurements.
4:54PM L9.00013 Direct measurements of the pair potentials of colloids with light scattering and optical traps, KISUN YOON, SEAS, Harvard University, VINOTHAN MANOHARAN, Department of Physics, SEAS, Harvard University — We present a methodology of directly measuring the pair potentials of colloids. We take snapshots of the thermal fluctuation of a pair of colloidal particles in equilibrium. The probability distribution of the separation distance obtained from the snapshots should follow the Boltzmann distribution because the separation distance of the particle pair is the only independent variable necessary to describe the effective free energy of a macrostate of the colloidal particle pair in equilibrium. The measurement of the pair potentials can be achieved by appropriately subtracting the unwanted potentials due to optical traps and optically induced interactions from the effective free energy. Accurate measurement of the separation distance between colloidal particles has critical importance in measuring colloidal interactions. Conventional Video Microscopy used for separation distance measurement is significantly restricted due to the two-dimensional nature of the measurement. Furthermore, the measurement is seriously distorted when the two particles are nearly in contact because of the diffraction of light and multiple scattering effect. We introduce a new technique to accurately measure the separation distances using light scattering. This light scattering technique can measure the separation distance in 3D and appropriately considers the multiple scattering effect.

5:06PM L9.00014 Concentration Gradients in Mixed Magnetic and Nonmagnetic Colloidal Suspensions, RANDALL ERB, BENJAMIN YELLEN, Duke University — The ability to form concentration gradients in mixed magnetic/nonmagnetic colloidal suspensions using magnetic field gradients has many practical applications in the fields of biosensors and life science diagnostics. Previously, we developed and experimentally confirmed a self-consistent model describing the local distribution of magnetic nanoparticles exposed to a magnetic field gradient. Here, we have derived an analytic expression to describe the local concentration of nonmagnetic colloids which are also affected by field gradients when inside magnetic colloidal suspensions. The model calculates the force on particles as a function of local magnetic particle concentration, and solves for the equilibrium distribution of particles through the drift-diffusion equations. We investigate the ability to concentrate and deplete nonmagnetic particles from specific regions of a substrate, such as nearby patterned micro-magnets on a substrate. Also, we have qualitative experimental results to support our expression. Our results show that nonmagnetic particles which are 5-10 times larger than the magnetic nanoparticles can be effectively concentrated or depleted at specified regions of the substrate.

5:18PM L9.00015 Interactions and self assembly of two heterogeneously charged surfaces, ROBERT BREWSTER, Dept. of Materials And Interfaces, Weizmann Institute of Science, PHILIP PINCUS, Dept. of Physics, SAMUEL SAFRAN, Dept. of Materials And Interfaces, Weizmann Institute of Science — Recent experiments1,2 have measured attractive interactions between two surfaces that each bear two molecular species with opposite charge. Theoretical considerations predict equilibrium finite-sized domains of each species, consistent with experiment. These domains, whose observed sizes are typically tens of nanometers, are the result of a balance between the line tension, which prefers macroscopic separation, and the electrostatics, which prefers mixing. Additionally, two such surfaces show a long range attraction. We present a theoretical model that predicts the domain size, phase behavior and forces for two such interacting surfaces.

Tuesday, March 11, 2008 2:30PM - 5:30PM —
Session L10 DMP: Focus Session: Electronic and Vortex Mechanisms for Higher Performing Superconductors Morial Convention Center RO8

2:30PM L10.00001 Exploring the limits of critical currents in superconductors, ALEX GUREVICH, National High Magnetic Field Laboratory, Tallahassee, FL 32310 — Mechanisms, which determine the ultimate limit of the critical current density \( J_c(T, B) \) in superconductors are discussed. The talk is mostly focused on the extreme strong pinning limit of highly deformed vortex segments, the role of anisotropy, current-blocking effects of pinning centers and grain boundaries, thermal fluctuations of vortices in high-\( T_c \) superconductors. In particular, the design of optimum pinning nanostructures, which produce the maximum \( J_c \), is addressed. The results are applied to YBCO thick-film coated conductors with insulating nanoprecipitates, for which several groups have reported very high \( J_c \), values, up to 12-20 % of the depairing current density. Requirements for a putative room-temperature superconductor to be useful in high-field applications are discussed.

3:06PM L10.00002 Current density in YBCO-based Tapes Studied over 8 Decades of Dissipation1, J.R. THOMPSON, Univ Tennessee & Oak Ridge Natl Lab, OZGUR POLAT, Univ. Tennessee, D.K. CHRISTEN, ORNL, D. KUMAR, NC A&T Univ, P.M. MARTIN, ORNL, J.W. SINCLAIR, Univ. Tennessee — Many applications of superconductors require conduction of high density electric currents in a magnetic field, with minimal dissipation. We investigated the dependence of current density \( J \) on electric field \( E \) due to motion of deformed vortices, over a range of \( 10^8 \) in \( E \). The materials are pre-commercial YBa\(_2\)Cu\(_3\)O\(_y\)-\( \gamma \) coated conductors (3.5\( \mu \)m) on buffered Hastelloy substrates prepared by SuperPower, Inc. Experimental methods include conventional 4-probe electrical transport at the highest \( E \) fields; inductive measurements of magnetic moment \( m \sim J \) using a swept magnetic field \( dH/dt \sim E \) at lower \( E \) fields; and time dependent “flux creep” measurement where \( dm/dt \sim E \). At \( T \approx 77 \) K, a power law variation \( E \sim J^\alpha \) is found. The resulting \( E(J) \) dependencies become steeper, i.e., the characteristic \( \alpha \) value increases, as \( J \) is reduced, reflecting a diverging activation energy for vortex movement. The inductive studies are easily extended to lower temperatures and a wide range of magnetic fields. Implications for applications will be discussed.

1 Research sponsored by DOE, Division of Materials Sciences and Engineering, and Office of Electricity Delivery and Energy Reliability.

3:18PM L10.00003 Isotropic critical currents in anisotropic superconductors: a simple physical model1, D.K. CHRISTEN, Y.L. ZUEV, S. WEE, A. GOYAL, S.W. COOK, Oak Ridge National Laboratory — Critical current densities, \( J_c \), that are nearly independent of magnetic field orientation can be observed in intrinsically anisotropic high-temperature superconductors that have specific, very strong flux pinning nanostructure. The phenomenon is observed to occur at specific temperature dependent fields, \( H^*(T) \). The possibility of such isotropic behavior can be described by a simple physical model based on the orientation dependence of the irreversibility field \( H_i(T, \theta) \) and the power-law decay exponent \( \alpha(\theta) \), where \( J_c \propto H_i^{\alpha(\theta)} \) in the intermediate field regime. An analysis will be discussed that elucidates necessary conditions for occurrence of the effect, and provides possible predictive tools for tailoring of \( H^*(T) \) to practical fields and temperatures by means of defect engineering.

1 Research sponsored by the U.S. Department of Energy - Office of Electricity Delivery and Energy Reliability and the Office of Science, Division of Materials Sciences and Engineering
3:30PM L10.00004 Exploring the limits to vortex pinning in superconductors\textsuperscript{1}, LEONARDO CIVALE, Los Alamos National Laboratory — Vortices in type II superconductors sit on a potential energy landscape created by material inhomogeneities. In the presence of an electrical current these inhomogeneities produce a restoring force that precludes vortex motion, thus allowing dissipation-free transport, as long as the current density does not exceed the critical current density $J_c$. Based on present theoretical understanding, by introducing the appropriate type of pinning centers it should be possible to attain $J_c$ values (for low vortex densities) as large as the physical limit determined by the depairing current density $J_0$. However, after decades of large efforts and resources dedicated to pinning enhancement (which has obvious technological relevance) we are far below that limit. Presently, the largest $J_c/J_0$ ratios have been obtained for very thin epitaxial $YBa_2Cu_3O_7$ films and are ~0.3, slightly higher than in the conventional superconductor Nb-Ti ($J_c/J_0 \sim 0.25$). I will analyze the possible reasons for this limitation and discuss possible ways to circumvent it. I will particularly focus on the influence of thermal fluctuations, which promote some level of vortex motion even below $J_c$, resulting in a temporal decay of the supercurrents and consequently lower $J_c$ values as determined by standard experimental techniques. Based on general principles, I will discuss what pinning performance we may expect in yet-to-be-discovered superconductors with high $T_c$.


4:06PM L10.00005 Magnetic field and temperature specific isotropic critical currents in strong-pinning high-temperature superconductors\textsuperscript{1}, Y.L. ZUEV, D.K. CHRISTEN, S.H. WEE, A. GOYAL, S.W. COOK, Oak Ridge National Laboratory — We report the observation of a unique temperature-dependent magnetic field, $H^*(T)$, at which the critical current of ($R$)BaCuO ($R$=rare earth) films with strong c-axis pinning can be nearly isotropic. That is, $J_c(\theta, H^*) \approx$ constant over nearly the entire interval of sample orientation from $H||c$ to $H||ab$ (in the full Lorentz force configuration). The phenomenon is observed in classes of HTS coatings that contain self-assembled, strongly pinning columnar stacks of second-phase precipitates, BaZrO$_3$, oriented near the $c$ axis, and appears to originate from the combination of and offsetting effects of material anisotropies. Systematics of this behavior will be explored and several important control parameters will be identified.

\textsuperscript{1}Research sponsored by the U.S. Department of Energy - Office of Electricity Delivery and Energy Reliability and by the Office of Science, Division of Materials Sciences and Engineering.

4:18PM L10.00006 AC losses in multifilamentary YBCO thin films, RAN YANG, ANDREA LUCARELLI, GUNTER LUEPKE, College of William and Mary, TIMOTHY HAUGAN, PAUL BARNES, AFRL Propulsion Directorate — Striation of superconducting tape allows the reduction of hysteresis losses. We studied the effect of an ac current as a function of the frequency and of a static magnetic field on the flux behavior in multifilamentary $YBa_2Cu_3O_7$ (YBCO) thin films. The current density, the magnetic and electric field profiles are determined quantitatively during the cycle. The shielding and transport current distribution in the filaments are affected by hysteresis and inductive effects that depend on the number and the distribution of the filaments. Time resolved magneto-optical imaging measurements reveal a cross-talk between adjacent conducting filaments that affects the overall hysteresis losses. This new, quantitative and fast method allows us to determine a of dynamic parameters, such as mapping the transport current density and electric field distribution during the ac cycle, that are important for practical superconducting applications and complementary to conventional transport measurement techniques.

4:30PM L10.00007 Evaluation of YBCO to 45T over wide temperature range, ZHIJUN CHEN, FUMITAKE KAMETANI, DAVID LARBALESTIER, Florida State University — The ability to tune the vortex pinning of YBCO in coated conductor form is both an enormous benefit to future superconducting materials applications and a challenge to understanding the properties over a broad range on particular samples. We have been doing such characterizations in support of the design of 30 T magnets. In recent work we have mapped the $J_c$ to fields of 35T at temperatures down to 4K and measured the angular dependent $J_c$ in similar fields. We see that it is possible to enhance $H_{c1}^*$ by about 15% as compared to standard YBCO at 55K, when a high density of RE$_2$O$_3$ nanoprecipitates is formed in the microstructure. These precipitate arrays produce $J_c$ of 50 MA/cm$^2$ almost 20% of the deparing current density.

4:42PM L10.00008 Vortex phases and dynamics in $YBa_2Cu_3O_7$+$BaZrO_3$ films as a function of angle and field up to 50 Tesla, S.A. BAILY, B. MAIOROV, H. ZHOU, S.R. FOLTYN, T.G. HOLESINGER, Q.X. JIA, LEONARDO CIVALE, Superconductivity Technology Center, LANL, Los Alamos, NM, F.F. BALAKIREV, M. JAIME, National High Magnetic Field Laboratory, LANL, Los Alamos, NM — Studying the vortex solid-liquid transition (nematic-0) in high $T_c$ superconductors is scientifically and technologically relevant. We have used low current transport measurements to study the melting line of $YBa_2Cu_3O_7$ films with and without $BaZrO_3$ additions in fields up to 50 T. Samples with mostly extended particle defects, mostly columnar defects, or a mixture of both will be compared. Plain $YBa_2Cu_3O_7$ shows correlated pinning along the crystalline axes and the emergence of a smectic phase when field is aligned with the a-b plane. Inclusion of $BaZrO_3$ not only alters the angular dependence of the irreversibility line indicating the stronger influence of c-axis correlated pinning, but also affects dissipation in the vortex-liquid state over the entire angular range. We will discuss the results in terms of vortex pinning, the corresponding types of phase transitions, micro-structural analysis, and information obtained from critical current measurements.

4:54PM L10.00009 Vortex pinning landscape in MOD-TFA YBCO nanostructured films, J. GUTIERREZ, T. PUIG, A. POMAR, X. OBRADORS, ICMAB-CSIC — A methodology of general validity to study vortex pinning in YBCO based on $J_c$ transport measurements is described. It permits to identify, separate and quantify three basic vortex pinning contributions associated to anisotropic-strong, isotropic-strong and isotropic-weak pinning centers. Thereof, the corresponding vortex pinning phase diagrams are built up. This methodology is applied to the new solution-derived YBCO nanostructured films, including controlled interfacial pinning by the growth of nanostructured templates by means of self-assembled processes [1] and YBCO-$BaZrO_3$ nanocomposites prepared by modified solution precursors. The application of the methodology and comparison with a standard solution-derived YBCO film [2], allows us to identify the nature and the effect of the additional pinning centers induced. The nanostructured templates films show c-axis pinning strongly increased, controlling most of the pinning phase diagram. On the other hand, the nanocomposites have achieved so far, the highest pinning properties in HTS-superconductors [3], being the isotropic-strong defects contribution the origin of their unique properties. [1] M. Gibert et al, Adv. Mat. vol 19, p. 3937 (2007) [2] Puig,T et al, SuST EUCAS 2007 (to be published) [3] J. Gutierrez et al, Nat. Mat. vol. 6, p. 367 (2007) * Work supported by HIPERCHEM, NANOARTIS and MAT2005-02047
5:06PM L10.00010 Flux dynamics in a two-band superconductor with delocalized electric fields. MILIND N. KUNCHUR, JAMES KNIGHT, Dept. of Physics & Astronomy, University of South Carolina — In conventional flux flow, vortex dissipation is localized to the vicinity of the vortex core leading to a viscous coefficient $\eta$ that is independent of flux density $B$ and a flux-flow resistance $R_f$ becomes independent of $B$, as observed in disordered magnesium diboride. Such an intrinsically field indifferent mixed-state response makes this system especially suited for magnetic-field induced switching.

Work supported by U. S. Department of Energy under grant no. DE-FG02-99ER45763.

5:18PM L10.00011 In-Field Critical Current by Correlated Anti-Pins in Type-II Superconductors. ERIC J. OSWALD, JOSE P. RODRIGUEZ, Physics & Astronomy, California State University at Los Angeles — The critical current shown by films of YBa$_2$Cu$_{3-x}$O$_y$ that contain naturally occurring linear pinning centers aligned parallel to the c-axis decays with increasing magnetic field that is also aligned in parallel as an inverse-square-root power law. Recent theoretical work based on 2D collective pinning of the vortex lattice by such material line defects recovers this dependence on magnetic field in the weak-pinning limit[1]. It further predicts an in-field critical current for correlated antipins that decays with magnetic field more slowly, as an inverse power law characterized by an exponent below 1/2. We test these predictions by performing Langevin dynamics simulations of the corresponding 2D vortex lattice driven by the Lorentz force. Long-range logarithmic interactions between vortices are assumed, while (anti)pinning centers are arranged in a "liquid" fashion. We find indeed that collective pinning by antipins result in a significant critical current. More detailed comparisons with theory in relation to the power-law decay with magnetic field will be made.


Tuesday, March 11, 2008 2:30PM - 5:30PM — Session L11 DCMP: Superconductivity: Transport and Fermi Pockets Morial Convention Center R09

2:30PM L11.00001 Low Temperature Thermal Conductivity in Cuprate Superconductors Amidst Coexisting Charge Order: Part II - Effect of Self-Consistent Disorder and Vertex Corrections. PHILIP SCHIFF, ADAM DURST, Stony Brook University — As in Part I, we consider a d-wave superconductor (dSC) in which the superconductivity coexists with charge density wave (CDW) order of wavevector $(\pi,0)$. Here we discuss two significant improvements to the calculation of the low temperature thermal conductivity. First, rather than taking the 4-by-4 self-energy matrix to be a scalar and a constant, independent of the CDW order parameter, we compute it from an impurity density and scattering potential, within the self-consistent Born approximation. We find that self-consistency requires two off-diagonal terms in the self-energy matrix, in addition to the diagonal term. Furthermore, we find that these off-diagonal terms dominate in the clean limit. Second, we include ladder corrections to the bare vertex, as required to satisfy Ward identities. We compute their contribution, which is verified to be small in the low impurity density limit. However, the contribution of the off-diagonal terms in the self-energy matrix is found to be quite important, significantly reducing the critical value of the CDW order parameter beyond which the thermal conductivity vanishes. Results are used to identify signatures of the effect of charge order on quasiparticle transport in the underdoped cuprates.

2:42PM L11.00002 Low Temperature Thermal Conductivity in Cuprate Superconductors Amidst Coexisting Charge Order: Part I - Bare Bubble Calculation. ADAM DURST, Stony Brook University, SUBIR SACHDEV, Harvard University — We consider a d-wave superconductor (dSC) in which the superconductivity coexists with charge density wave (CDW) order of wavevector $(\pi,0)$. While the nodes of the quasiparticle energy spectrum survive the onset of charge order, there exists a critical value of the CDW order parameter beyond which the quasiparticle spectrum becomes fully gapped. We perform a linear response Kubo formula calculation of thermal conductivity in the low temperature (universal) limit, where a simplified model of disorder has been employed and vertex corrections have been neglected. Effects of self-consistent disorder and vertex corrections are discussed in a separate talk — Part II. Results reveal the dependence of thermal transport on increasing CDW order parameter up to the critical value at which the quasiparticle spectrum becomes fully gapped and thermal conductivity vanishes. In addition to numerical results, closed-form expressions are obtained in the clean limit for the special case of isotropic Dirac nodes.

2:54PM L11.00003 Thermal and electrical transport in a random dissipative quantum system controlled by an infinite randomness critical point. ADRIAN DEL MAESTRO, BERND ROSENOW, MARKUS MUELLER, SUBIR SACHDEV, Harvard University — The complicated interplay between quantum fluctuations and disorder in the vicinity of a quantum phase transition can have drastic effects and lead to exotic Griffiths phases and the flow to infinite randomness. We present a study of a dissipative Hertz-like theory in the presence of quenched disorder which may describe the quantum phase transition between a superconductor and metal in ultra narrow metallic wires tuned by an external source of pair-breaking. By finding a numerical solution to the large-N self-consistency equations for real-space chains we are able to directly compute the finite temperature thermal and electrical correlating through the quantum critical regime. From an analysis of the typical and average correlation functions we find evidence for dynamically activated scaling in accord with recent strong disorder real space renormalization group calculations.

3:06PM L11.00004 Theory of the Marginal Fermi liquid. ARKADY SHEETER, CHANDRAVARMA, UC Riverside — Marginal Fermi liquid is a successful phenomenological description of the strange metallic phase of cuprates near optimal doping. We cast the theory into the standard microscopic form for interacting fermions, employing particle-hole scattering and (singular) Landau parameters. We calculate the density-density correlation function and demonstrate its standard relation to the conductivity through the continuity equation. Internal consistency of the theory is ensured by showing that the relevant conservation laws are obeyed. The relation to the kinetic equation is established.

A.S. is partially supported by I2CAM award from NSF Grant DMR # 0645461.

3:18PM L11.00005 The effect of electron pockets on the quasiparticle interference patterns in cuprate. KANGJUN SEO, JIANGPING HU, Purdue University — We study the hole/electron pockets in the d-density wave and the spin density wave states. While the hole/electron pockets can be seen in the presence of the DDW and the SDW orders, the shape, locations, and the number of the Fermi pockets are different, depending on the band structures and the wavevectors of the order parameters. We calculate the local density of states in the presence and the absence of the electron pockets in the DDW and SDW states. We find that the quasiparticle scattering interference patterns by the single impurity are dramatically affected in the presence of the DDW and SDW order in comparison with one without the electron pockets.
3:30PM L11.00006 Quantum oscillations and Fermi surface in underdoped YBa$_2$Cu$_3$O$_{6.5}$, N. DOIRON-LEYRAUD, Universite de Sherbrooke, CYRIL PROUST, LNCP Toulouse, DAVID LEBOEUF, Universite de Sherbrooke, JULIEN LEVALLOIS, LNCP Toulouse, JEAN-BAPTISTE BONNEMAISON, Universite de Sherbrooke, RUIXING LIANG, DOUG BONN, WALTER HARDY, University of British Columbia and CIAR, LOUIS TAILLEFER, Universite de Sherbrooke and CIAR — We report quantum oscillations in the transport properties of YBa$_2$Cu$_3$O$_{6.5}$ at 10% doping, showing that a well-defined Fermi surface with closed orbits is a fundamental property of underdoped cuprates. In contrast with the large Fermi surface seen on the overdoped side, we observe a very small orbit whose area is only 1.9% of the Brillouin zone. Such a small Fermi surface does not come from the band structure of YBa$_2$Cu$_3$O$_{6.5}$ and is most likely the result of a reconstruction.

3:42PM L11.00007 Shubnikov-de Haas oscillations in YBa$_2$Cu$_3$O$_y$, A. F. BANGURA, J. D. FLETCHER, A. CARRINGTON, P. J. HEARD, N.E. HUSSEY, (Bristol), J. LEVALLOIS, M. NARDONNE, B. VIGNOLLE, C. PROUST, (LNCP, Toulouse), N. DOIRON-LEYRAUD, D. LEBOEUF, T. TAILLEFER, (Sherbrooke), S. ADACHI, (ISTEC, Tokyo) — The recent report of quantum oscillations in the single-chain underdoped cuprate YBa$_2$Cu$_3$O$_{6.5}$ - ortho II (hole doping $p < 0.10$) points to the possibility that the underlying electronic structure in the underdoped region of the cuprate phase diagram contains Fermi surface pocket(s), at odds with results from ARPES experiments. In this talk I will describe our observation of quantum oscillations in the Hall resistivity $\rho_{xy}$ of the stoichiometric double-chain cuprate YBa$_2$Cu$_3$O$_y$ (hole doping $p < 0.14$), in pulsed magnetic fields up to 62T. Our results show that both the area of the quasiparticle orbit and the cyclotron effective mass of YBa$_2$Cu$_3$O$_6$ are larger than those measured for YBa$_2$Cu$_3$O$_{6.5}$ - ortho II. The observed negative Hall coefficient and the failure of LDA bandstructure calculations to account for the oscillations suggests a non-trivial origin. However, clear evidence of quantum oscillations in materials with such different levels of doping and of the details of the transport properties of the two compounds, allows us to conclude that small Fermi surface pocket(s) are a generic feature of the underdoped side of the Yttrium-based cuprate phase diagram and are associated with the CuO$_2$ planes.

3:54PM L11.00008 Electron pockets in the Fermi surface of hole-doped high-Tc superconductors, DAVID LEBOEUF, NICOLAS DOIRON-LEYRAUD, JULIEN LEVALLOIS, RAMZY DAOU, B. BONNEMAISON, NIGEL HUSSEY, LUIS BALICAS, BRAD RAMSHAW, RUIXING LIANG, DOUG BONN, WALTER HARDY, S. ADACHI, CYRIL PROUST, LOUIS TAILLEFER — The Fermi surface of the electronic states in the underdoped YBCO materials YBa$_2$Cu$_3$O$_y$ and YBa$_2$Cu$_4$O$_8$ was recently shown to include small pockets, in contrast with the large cylinder that characterizes the overdoped regime, pointing to a topological change in the Fermi surface. Here we report the observation of a negative Hall resistance in the magnetic-field-induced normal state of YBa$_2$Cu$_3$O$_y$ and YBa$_2$Cu$_4$O$_8$, which reveals that these pockets are electron-like rather than hole-like. We propose that these electron pockets most probably arise from a reconstruction of the Fermi surface caused by the onset of a density-wave phase, as is thought to occur in the electron-doped copper oxides near the onset of antiferromagnetic order.

4:06PM L11.00009 Evidence of Fermi surface reconstruction and the formation of small hole pockets in underdoped La$_{2-x}$Sr$_x$CuO$_4$: Far Infrared Hall measurements, D.C. SCHMADEL, G.S. JENKINS, H.D. DREW, CNAM, University of Maryland at College Park, I. TSUKADA, T. ANDO, Materials Science Research Laboratory, CRIEPI, Tokyo, Japan — The Hall effect in La$_{2-x}$Sr$_x$CuO$_4$ films is measured from 3 to 100 meV as a function of temperature from 5K to 300K and carrier doping ranging from severely underdoped ($x = 0.03$) to optimal doped ($x = 0.15$). The behavior of the infrared Hall angle with temperature and frequency is found to be consistent with a simple extended Drude model at all dopings. A significant reduction of the Hall mass is observed when the hole doping level is reduced from optimal doping, which is consistent with a drastic reduction of the Fermi surface volume. These results are similar to earlier mid-IR Hall measurements obtained in underdoped YBCO. [1] and are related to the recent observation of quantum oscillations reported in YBCO. [2]


The authors acknowledge support of the NSF through grants DMR-0303112.

4:18PM L11.00010 Evidence of Fermi surface reconstruction in Pr$_{2-x}$Ce$_x$CuO$_4$: Far IR Hall measurements in electron doped cuprates, G.S. JENKINS, D.C. SCHMADEL, P. BACH, R.L. GREENE, H.D. DREW, University of Maryland at College Park, CNAM, UNIVERSITY OF MARYLAND AT COLLEGE PARK — The Hall Effect is measured at far infrared frequencies (24-85 1/cm) in Pr$_{2-x}$Ce$_x$CuO$_4$ films as a function of temperature from 5K to 300K and electron doping levels ranging from severely underdoped ($x = 0.10$) to overdoped ($x = 0.19$). In underdoped PCCO, the doping and temperature dependence of the complex Hall angle is found to be consistent with a simple Drude model with an associated reduction of the Hall mass in comparison with optimal doping. The mass reduction is consistent with Fermi surface reconstruction and the formation of small electron pockets. In overdoped PCCO, evidence for both electron and hole contributions to $\sigma_{xy}$ is observed even at low temperatures, a contradictitious result compared with the DC Hall Effect in PCCO as well as the behavior observed in IR Hall measurements in La$_{2-x}$Sr$_x$CuO$_4$. These data suggest interactions through the exchange of incoherent zone corner magnons.

The work was supported by NSF grants DMR-0303112 and DMR-0653535.

4:30PM L11.00011 Disorder and the Metal-Insulator Crossover in Pr$_{2-x}$Ce$_x$CuO$_{1-y}$, P. L. BACH, W. YU, J. S. HIGGINS, H. XU, R. L. GREENE, CNAM, Department of Physics, University of Maryland, B. WEAVER, Naval Research Laboratory — One of the outstanding issues in the electron doped cuprates is the role that oxygenation plays in the superconductivity and normal state properties. Oxygen addition can be considered both a doping and a disordering process. To disentangle these two effects, disorder can be introduced by irradiating the samples without altering doping. We report transport studies on optimal and underdoped Pr$_{2-x}$Ce$_x$CuO$_{1-y}$ films subject to proton irradiation and oxygenation. We establish a correlation between the static AFM and the metal-insulator crossover. Our separation of the disorder and doping effects also shed light on oxygen reduction effects in electron-doped cuprates. Supported by NSF grant DMR-0653535.

4:42PM L11.00012 Doping dependence of the dynamic critical exponent in Pr$_{2-x}$Ce$_x$CuO$_4$, M.C. SULLIVAN, J. SOUSA, M. SALVAGGIO, Department of Physics, Ithaca College, Ithaca NY, R.L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland. College Park — Scaling analysis of voltage vs. current isotherms is a favorite tool to study the normal-superconducting phase transition in cuprate superconductors. This measurement has never been performed on the electron-doped cuprate superconductor Pr$_{2-x}$Ce$_x$CuO$_4$, despite unusual behaviors which may alter this phase transition and yield interesting results (behaviors such as the extended doping range of the antiferromagnetic phase and the quantum critical point). This is perhaps due to the lack of consensus regarding the analysis of voltage vs. current isotherms, due in part to finite-thickness effects even in thick ($d \approx 3000\AA$) films. If finite-thickness effects are taken into consideration, we can find the dynamic critical exponent $z$ in our Pr$_{2-x}$Ce$_x$CuO$_4$ films. We present our results of the dynamic critical scaling exponent $z$ as a function of doping.

Supported by NSF grant DMR-0706557.

4:54PM L11.00013 Thermal and electrical transport in the cuprate superconductor Nd-LSCO. 
LOUIS TAILLEFER, R. DAOU, S.Y. LI, DAVID LEBOEUF, OLIVIER CYR-CHONIERE, University of Sherbrooke, J.-Q. YAN, J.-S. ZHOU, J.B. GOODENOUGH, University of Texas at Austin — We present a study of the thermal and electrical transport properties of the cuprate superconductor Nd-LSCO in a wide range of doping from x=0.12 to x=0.25. The behavior of the thermal conductivity in the zero temperature limit allows us to access the quasi-particle transport in both the superconducting and normal state. The impact of stripe order on quasiparticle transport is discussed.

5:06PM L11.00014 Measurements of the Hall Effect and Resistivity in La_{2-x}Sr_{x}CuO_{4+δ} with Ultrafine Stoichiometry Resolution, $\delta x \sim 2.5 \times 10^{-4}$. JEFFREY CLAYHOLD, BRYAN KERNS, MICHAEL SCHROER, DAVID RENCH, Physics Department, Miami University, GENNADY LOGVENOV, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory — Recent reports of sharp changes of transport properties with small variations of stoichiometry in cuprate superconductors have motivated us to look for similar behavior in optimally- and over-doped La_{2-x}Sr_{x}CuO_{4+δ}, using a recently completed system for creating and measuring samples with ultrafine stoichiometry resolution. The data are from MBE films grown with a linear stoichiometry gradient and were taken with a characterization system that can measure both the Hall effect and resistivity simultaneously at 31 different locations on the film. We will show new data for x ranging from 0.15 to 0.30.

5:18PM L11.00015 Magnetotransport and noise in lightly doped La_{2−x}Sr_{x}CuO_{4} and La_{2}Cu_{1−x}Li_{x}O_{4}. IVANA RAICIEVIC, Dept. of Physics and National High Magnetic Field Laboratory (NHMFL), Florida State Univ. (FSU), DRAGANA POPOVIC, NHMFL/FSU, CHRISTOS PANAGOPoulos, Cavendish Laboratory, Univ. of Cambridge, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology — We report a detailed comparative study of magnetotransport and noise in high quality single crystals of La_{2-x}Sr_{x}CuO_{4} (LSCO) and La_{2}Cu_{1-x}Li_{x}O_{4} (x = 0.03) at temperatures 0.100 < T(K) < 150 and fields 0 < B(T) < 18 parallel and perpendicular to the c-axis. Our results demonstrate that, in both materials at low T, the positive magnetoresistance (MR) exhibits signatures of glassiness, such as hysteretic behavior and memory. At such low T < T_{sg} (T_{sg} = spin glass transition temperature), the resistance noise data reveal other glassy features, such as slowing down of the charge dynamics and the onset of cooperativity at T is reduced. The crossover to negative MR takes place at higher T and B in all samples and for both B orientations. However, for B || c, a steep decrease in MR is observed only in La_{2}Cu_{1-x}Li_{x}O_{4} at high T, as the system enters the Néel state, similar to the result obtained on antiferromagnetic LSCO with x = 0.01 [1]. [1] Supported by NSF DMR-0403491, NHMFL via NSF Grant DMR-0084173, and The Royal Society.

2:30PM L12.00001 Phonon Anomalies in α-uranium. XIADONG YANG, PETER RISEBOROUGH, Temple University — The temperature-dependence of the phonon spectrum of α-uranium has recently been measured by Manley et al. [1] using inelastic neutron scattering and x-ray scattering techniques. Although there is scant evidence of anharmonic interactions, the phonons were reported to show some softening of the optic modes at the zone boundary. The same group of authors later reported that an extra mode was observed to form at a temperature above 450 K [2]. The existence of the proposed new mode is inconsistent with the usual theory of harmonic phonons, as applied to a structure composed of a monoclinic Bravais lattice with a two-atom basis. We investigate the effect that the f electron-phonon interaction has on the phonon spectrum and its role on the possible formation of a breathing mode of mixed electronic and phonon character.

Work supported by the US Department of Energy, Office of Basic Energy Sciences.

2:42PM L12.00002 Phonon Spectra and Lattice Thermal Conductivity of UO2 and PuO2. QUAN YIN, SERGEY SAVRASOV, University of California, Davis — Electronic structure, phonon spectrum and lattice thermal conductivity of UO2 and PuO2 are studied using a combination of Density Functional Theory within Local Density Approximation and Dynamical Mean Field Theory (LDA+DMFT). UO2 and PuO2 are mixed oxides fuel (MOX) used in modern thermal reactors. Both oxides are Mott-insulators with strongly correlated 5f electrons, showing very similar electronic structures and phonon dispersions. The calculated phonon dispersion for UO2 is generally consistent with experiment and we give prediction and PuO2 are mixed oxides fuel (MOX) used in modern thermal reactors. Both oxides are Mott-insulators with strongly correlated 5f electrons, showing very similar electronic structures and phonon dispersions. The calculated phonon dispersion for UO2 is generally consistent with experiment and we give prediction when the proposed experiment is consistent with the usual theory of harmonic phonons, as applied to a structure composed of a monoclinic Bravais lattice with a two-atom basis. We investigate the effect that the f electron-phonon interaction has on the phonon spectrum and its role on the possible formation of a breathing mode of mixed electronic and phonon character.


2:54PM L12.00003 Spectral Properties of Plutonium and its Compounds. JIAN-XIN ZHU, Los Alamos National Laboratory, A.K. MCMAHAN, Lawrence Livermore National Laboratory, M.D. JONES, University at Buffalo, SUNY, T. DURAKIEWICZ, J.J. JOYCE, J.M. WILLS, R.C. ALBERS, Los Alamos National Laboratory — By combining the local density approximation (LDA) with dynamical mean field theory (DMFT), we analyze the spectral properties of plutonium and its compounds. The LDA Hamiltonian is extracted either from a tight-binding fit to full-potential linearized augmented plane-wave calculations, or directly from the full-potential linearized muffin tin orbitals calculations. The DMFT equations are solved by the exact quantum Monte Carlo method complemented with the Hubbard-I approximation. We compare the f electron behaviors in Pu elemental solid and compounds. The theoretical results will also be discussed in the context of photoemission spectroscopy data.

3:06PM L12.00004 Crossover from non-Fermi liquid to Fermi liquid behavior: Amplitude of de Haas-van Alphen oscillations. PEDRO SCHLOTTMANN, Florida State University — Deviations from Landau’s Fermi liquid behavior in numerous U, Ce and Yb based heavy fermion systems are known as non-Fermi liquid behavior and are frequently attributed to a quantum critical point (QCP). A nested Fermi surface together with the remaining interaction between carriers after the heavy bands are formed may give rise to itinerant antiferromagnetism. We consider an electron pocket and a hole pocket, with Fermi momenta $k_{F1}$ and $k_{F2}$, respectively. The order can be suppressed by increasing the mismatch of the Fermi momenta and a QCP is obtained as $T_{N} \rightarrow 0$. For the tuned QCP the specific heat over $T$ increases as the logarithm of the temperature as $T$ is lowered [1] and the linewidth of the quasi-particles is linear in $T$ and $\omega$. [2] The numerical results display a crossover from non-Fermi liquid ($\sim T$) to Fermi liquid ($\sim T^{2}$) behavior. [2] Using the quasi-particle linewidth the temperature dependence of the amplitude of the de Haas-van Alphen oscillations (corresponding to the pocket frequencies) is computed.


3:06PM L12.00004 Crossover from non-Fermi liquid to Fermi liquid behavior: Amplitude of de Haas-van Alphen oscillations. PEDRO SCHLOTTMANN, Florida State University — Deviations from Landau’s Fermi liquid behavior in numerous U, Ce and Yb based heavy fermion systems are known as non-Fermi liquid behavior and are frequently attributed to a quantum critical point (QCP). A nested Fermi surface together with the remaining interaction between carriers after the heavy bands are formed may give rise to itinerant antiferromagnetism. We consider an electron pocket and a hole pocket, with Fermi momenta $k_{F1}$ and $k_{F2}$, respectively. The order can be suppressed by increasing the mismatch of the Fermi momenta and a QCP is obtained as $T_{N} \rightarrow 0$. For the tuned QCP the specific heat over $T$ increases as the logarithm of the temperature as $T$ is lowered [1] and the linewidth of the quasi-particles is linear in $T$ and $\omega$. [2] The numerical results display a crossover from non-Fermi liquid ($\sim T$) to Fermi liquid ($\sim T^{2}$) behavior. [2] Using the quasi-particle linewidth the temperature dependence of the amplitude of the de Haas-van Alphen oscillations (corresponding to the pocket frequencies) is computed.


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Although ferromagnetic ordering does occur in some materials, such as CeRu2Ge2. Extending a previously developed framework [1] for the antiferromagnetic Kondo lattice, we now consider the case where the magnitude of the antiferromagnetic Kondo coupling is small compared to the ferromagnetic RKKY interactions. The magnetic orderings in spin waves and conduction electrons are relevant, resulting in a change in the form of the QNLsM in the appropriate energy and momentum range. At the lowest energies, a gap in the continuum of excitations renders the Kondo coupling irrelevant. We conclude that a ferromagnetic state with a "small" Fermi surface (where local moments are not included in the Fermi volume) is stable. Finally, we discuss how the lack of Kondo screening in magnetic materials is reflected in magnetic properties. We show that, in some cases, spin symmetry breaking does not lead to a reduction of spin symmetry, further emphasizing the need to go beyond the conventional order parameter to characterize these magnetic quantum phases. [1] S. J. Yamamoto and Q. Si, Phys. Rev. Lett. 99, 016401 (2007)

3:42PM L12.00007 Study of the gap formation in Kondo insulators. M. A. MAJIDI, University of North Dakota, K. MIKELSONS, A. MACRIDIN, University of Cincinnati, J. MORENO, University of North Dakota, M. JARRELL, University of Cincinnati — Motivated by recent experimental measurements of the temperature-dependent gap formation in the Kondo insulator SmB6 (Matsunami et al.) we investigate the periodic Anderson Model at half-filling and in the strong-coupling regime. We solve this model in three dimensions using the Dynamical Cluster Approximation to incorporate non-local correlations and the Maximum Entropy Method to derive the spectral functions. We calculate the temperature dependence of the insulating gap and the screened moment, and discuss how the appearance of the gap is related with the lattice Kondo screening.

3:54PM L12.00008 Is FeSi a Kondo Insulator? JAN KUNES, University of Augsburg, VLADIMIR I. ANISIMOVA, Institute of Metal Physics, Yekaterinburg — Using combination of a simple model of local bandstructure and quantum Monte-Carlo technique we show that 3d 'Kondo insulators' such as FeSi and FeSb differ in many respects from classical f-electron based Kondo insulators. In particular we show that hybridization between narrow f-band and a broad conduction band typical for f-electron compounds is not a necessary condition for observation of the typical Kondo insulator behavior of susceptibility and dc as well as ac conductivity. The difference between FeSi and f-electron Kondo insulators becomes apparent when doped, while the former exhibits enhanced susceptibility leading to a Stoner-like ferromagnetic instability the latter are usually characterized by competition between the Kondo screening and local moment magnetism with RKKY inter-site coupling.

4:06PM L12.00009 A Phenomenological Theory of Quantum Tricritical Point: Applications to a Heavy-Fermion Compound YbRh2Si2. TAKAHIRO MISAWA, Department Applied Physics, Univ. of Tokyo, YOUHEI YAMAJI, MASATOSHI IMADA — We construct a phenomenological theory of quantum tricritical point (QTPC) of itinerant antiferromagnets by extending the self-consistent renormalization theory. We have shown that a novel non-Fermi liquid behavior comes out at the QTPC where a continuous phase transition changes into a first-order one at zero temperature. In contrast to the conventional quantum criticality proposed by Moriya, Hertz and Millis, a remarkable feature of the QTPC is the divergence of the ferromagnetic susceptibility at the antiferromagnetic phase transition under the magnetic field. In a heavy-fermion compound YbRh2Si2, enhancement of the ferromagnetic susceptibility near the antiferromagnetic quantum critical point has been an unsolved puzzle. We have shown that the quantum tricriticality naturally explains this puzzling enhancement. In particular, singularities of ferromagnetic susceptibility and the magnetization curve near the QTPC are well consistent with the experimental results.

4:18PM L12.00010 Two Channel Kondo Effect and Superconductivity in Pu and Np compounds. REBECCA FLINT, MAXIM DZERO, PIERS COLEMAN, Rutgers University — Recently, superconductivity has been observed in two heavy fermion compounds, PuCoGa4 and NpPdAl2, which transition directly from unquenched spins into the superconducting state, without passing through an intermediate heavy fermi liquid state. These two compounds can be modeled with the two channel Kondo model, where the two channels derive from virtual valence fluctuations of different crystal symmetries. The electron-spin scattering develops an Andreev component, creating a composite bound state of a spin-flip and a triplet pair of electrons. This process can be examined in a controlled fashion with symplectic N, with the maximum transition temperature occurring when the two channels have equal strengths. We will also discuss the effect of Pu doping on the superconducting transition temperature of NpPdAl2.

4:30PM L12.00011 Fermionic quantum criticality and the fractal nodal surface. FRANK KRUGER, JAN ZAANEN, Institut-Lorentz, Leiden University — Normal metals are characterized by a degeneracy scale imposed by Fermi-Dirac statistics: the Fermi energy. This paradigm breaks down in the high-Tc and heavy-fermion compounds where one encounters metallic states with scale invariant quantum dynamics. A theoretical understanding of these quantum critical states is lacking because the fermionic minus signs render the path integral non-probablistic. We demonstrate that within the constraint-path-integral formalism scale invariance and Fermi-Dirac statistics can be reconciled. The latter is translated into a geometrical constraint structure. We prove that this "nodal hypersurface" encodes the scales of the Fermi liquid and turns fractal when the system becomes quantum critical. To illustrate this we calculate nodal surfaces and electron momentum distributions of Feynman backflow wave functions and indeed find that with increasing backflow strength the quasiparticle mass gradually increases, to diverge when the nodal structure becomes fractal. This explains precisely the puzzling behaviors observed in the heavy-fermion intermetallics.

4:42PM L12.00012 Non-linear Sigma Model of Kondo Lattice in Antiferromagnetic Regime. TZEN ONG, Stanford University, B. A. JONES, IBM Almaden Research Center — We analyze the antiferromagnetic transition in heavy fermion compounds in two dimensions, which is studied in this paper, to be in the antiferromagnetic regime, with a Heisenberg coupling (Jzz) that is larger than the Kondo coupling (JK). The Heisenberg terms are mapped onto a non-linear sigma model, and the fermions are then formally integrated out to obtain an effective theory for the Neel field. We then study the evolution of the Heisenberg and Kondo couplings under perturbative RG, and calculate the critical exponents at the phase transition. Preliminary results indicate the possibility of a quantum phase transition from an AFM to a helical phase with anisotropy in the time-like direction.
Derivation and study of the Fermi-Majorana bi-resonant level model. C. J. BOLECH, Rice University, A. IUCCI, University of Geneva — We review the mapping of the anisotropic two-channel Anderson impurity model to a Fermi-Majorana bi-resonant level model. The correspondence is rigorously proved by using bosonization and explicitly constructing the new fermionic fields and Klein factors in terms of the original ones. We also demonstrate that the fixed points associated to the solvable manifold of the new model are renormalization-group stable and generic, and therefore representative of the physics of the original isotropic model. The simplicity of the mapped model allows for the computation of the full set of thermodynamic quantities as well as the identification of the different physical energy scales. In the absence of external fields the impurity physics is of non-Fermi liquid type. As expected, an arbitrarily small external field breaks some of the symmetries and introduces an extra energy scale below which the system flows to a local Fermi-liquid fixed point.

Tuesday, March 11, 2008 2:30PM - 5:18PM –
Session L13 DCOMP: Ground State Density Functional Theory: Theory Development

2:30PM L13.00001 Strictly correlated electrons in density-functional theory: A general formulation with applications to spherical densities, MICHAELA SEIDL, Institute of Theoretical Physics, University of Regensburg, Germany — We reformulate the strong-interaction limit of electronic density functional theory in terms of a classical problem with a degenerate minimum. This allows us to clarify many aspects of this limit, and to write a general solution which is explicitly calculated for spherical densities. We then compare our results with previous approximate solutions and discuss the implications for density functional theory.

2:42PM L13.00002 Spherically and system-averaged pair densities in the strong-interaction limit of density functional theory, PAOLO GORI-GIORGI, ANDREAS SAVIN, Laboratoire Chimie Théorique, CNRS and University Paris VI, Paris, France, MICHAELA SEIDL, Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — The spherically and system-averaged pair density (also known in chemistry as intracule density) plays a central role in the construction and understanding of exchange-correlation energy functionals in density functional theory. We have calculated the intracule density for several atoms in the strong-interaction limit of density functional theory. Comparison of our results with the same quantities calculated in the opposite limit, the non-interacting Kohn-Sham system, provides useful insight on the nature of electronic correlation in density functional theory.

2:54PM L13.00003 Internally Consistent Local Approximation to Density Functional Theory, ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We propose a new non-local functional for the implementation of density functional theory (DFT) within a local approximation. This functional is obtained through the replacement of the conventional form $T_\alpha = \frac{1}{2} \int \frac{d\mathbf{r}'}{n_\alpha} \int \frac{d\mathbf{r}_1}{n_\alpha} \frac{n_\alpha(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}')}{n_\alpha(\mathbf{r}_1) n_\alpha(\mathbf{r}_2)}$ to represent the kinetic and Coulomb energy of a non-interacting system with the expression $T_\alpha = \frac{1}{2} \int \frac{d\mathbf{r}_1}{n_\alpha(\mathbf{r}_1)} \int \frac{d\mathbf{r}_2}{n_\alpha(\mathbf{r}_2)} n_\alpha(\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}')$, where $n_\alpha(\mathbf{r})$ is the two-particle density formed from the non-interacting wave function, and $n_\alpha(\mathbf{r})$ is the single-particle density. Based on this new functional we develop a local approximation and show that it is self-interaction free and also leads to energies that form an upper bound to the exact ground-state energy. We provide a brief comparison with the conventional Kohn-Sham local density approximation and some of the schemes introduced to correct for the presence of self-interaction in the conventional formalism, and comment on our immediate plans for future development.


3:18PM L13.00005 The Role of Quantum Stress in Descriptive Chemistry, ILYA TOKATLY, Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Germany, GIOVANNI VIGNALE, University of Missouri-Columbia, JIANMIN TAO, Los Alamos National Laboratory — We show that key concepts of descriptive chemistry, such as atomic shells, bonding electron pairs and lone electron pairs, may be described in terms of quantum stress focusing, i.e. the spontaneous formation of closed surfaces upon which the electronic pressure has an extremum. This description subsumes previous mathematical constructs, such as the Laplacian of the density and the electron localization function, and provides a new tool for visualizing chemical structure. We also show that the full anisotropic stress tensor can be easily calculated from density functional theory.

3:30PM L13.00006 Semiclassical Approaches in Density Functional Theory, PETER ELLIOTT, ATTILA CANGI, DONGHYUNG LEE, KIERON BURKE, University of California, Irvine — We discuss the use of semiclassical methods in understanding, and improving, density functional theory (DFT). It has been found[1] that semiclassical approaches can explain many features of modern exchange-correlation approximations, such as the local density approximation or generalized gradient approximations. In this work, we continue this line of inquiry, showing how semiclassical approximations may be used to construct a form for the non-interacting kinetic energy density. A semiclassical approximation to the Green’s function is made[2], which, when integrated appropriately, yields leading corrections to the Thomas-Fermi result. It can be regarded as a functional of the potential. We test this approximation for various 1D systems confined within a box and present the results. This, coupled with the corresponding form of the density[2], could provide an orbital-free DFT which would allow more complex systems to be studied.


3:42PM L13.00007 Correlation Energy of 3D Spin-Polarized Electron Gas: A Single Interpolation Between High- and Low-Density Limits. JIAWEI SUN, JOHN PERDEW, Department of Physics and Quantum Theory Group, Tulane University, MICHAEL SEIDL, Department of Physics, University of Regensburg. — We present an analytic model for the correlation energy per electron \( N_e \left( \varepsilon \right) \) in the three-dimensional (3D) uniform electron gas, covering the full range \( 0 \leq \varepsilon \leq \infty \) and \( 0 \leq \zeta \leq 1 \) of the density parameter \( r_s \) and the relative spin polarization \( \zeta \). An interpolation is made between the exactly known high-density (\( r_s \to 0 \)) and low-density (\( r_s \to \infty \)) limits, using a formula which (unlike previous ones) has the right analytic structures in both limits. We find that there is almost enough information available from these limits to determine the correlation energy over the full range. By minimal fitting to numerical quantum Monte Carlo data, we predict the value of \( b_1(\zeta) \) at \( \zeta = 0 \) close to the theoretical value [1], where \( b_1(\zeta) \) is the coefficient of the \( r_s \) term in the high-density expansion. The model finds correlation energies for the unpolared \( (\zeta = 0) \) and fully polarized \( (\zeta = 1) \) cases in excellent agreement with Monte Carlo data.


3:54PM L13.00008 Semiclasiﬁc Origin of Density Functionals. ATTILA CANGI, PETER ELLIOTT, DONGHYUN LEE, KIERON BURKE, University of California, Irvine. — We use methods of semiclassical physics [1] to study the basic ingredients of DFT in terms of an asymptotic expansion in powers of the particle number. As an example we derive an approximate many-particle density [2] of a general potential in a one-dimensional system with hard walls. If the Fermi wave number lies above the maximum of the potential, we obtain densities very close to the exact answer, even for a small particle number. Density oscillations due to the effect of the boundaries are also present.


4:06PM L13.00009 Construction of an analytic exchange-correlation hole for the Penderwe-Burke-Ernzerhof GGA. MATTHIAS ERNZERHOF, Department of Chemistry, University of Montreal, HILKE BAHMANN, Department of Chemistry, University of Wuerzburg. — The Perdew-Burke-Ernzerhof (PBE) [1] approximation to the exchange-correlation energy is employed as a starting point for the construction of an approximate, spherically averaged exchange-correlation hole. In a first step, we develop a new model for the PBE exchange hole. This model satisfies the homogeneous electron gas limit; it is normalized and yields the correct small-gradient limit in the system average. A correlation factor [2], i.e., a function multiplying the exchange hole, is proposed that turns the exchange into an exchange-correlation hole. The correlation factor has a simple form and its parameters are determined through a number of known conditions that are satisfied by a PBE exchange-correlation hole. The homogeneous-electron-gas limit of the new hole model is compared to the LSD hole [3].


4:18PM L13.00010 Orbital-free Kinetic Energy Density Functional of GGA Type with Positive-definite, Finite Pauli Potentials. S.B. TRICKEY, QTP, Univ. Florida, V.V. KARASIEV, Instituto Venezolano de Investigaciones Cientificas, R.S. JONES, Physics, Loyola College of Maryland, FRANK HARRIS, Physics, Univ. Utah. — A reliable, orbital-free expression for the Kohn-Sham kinetic energy functional \( T_{KS} \) would provide Born-Oppenheimer forces of first-principle many-particle density [2] of general potential in a one-dimensional system with hard walls. If the Fermi wave number lies above the maximum of the potential, we obtain densities very close to the exact answer, even for a small particle number. Density oscillations due to the effect of the boundaries are also present. Illustrative results will be reported.

1Work supported in part by US NSF ITR Grant DMR-0325553.

4:30PM L13.00011 Exact condition on the non-interacting kinetic energy for real matter. DONGHYUN LEE, KIERON BURKE, University of California, Irvine. — From the analysis of the asymptotic expansion [1,2] for the total energies of neutral atoms, we suggest a modified gradient expansion approximation to the kinetic energy which satisfies the exact asymptotic condition as the number of electrons \( N \to \infty \). The resulting function determines the small gradient limit of any generalized gradient approximation, and conflicts with the standard gradient expansion. We apply this new functional to the atoms up to \( Z \to 88 \) in comparison with the 2nd and 4th gradient expansion approximations. We also give a modern, highly accurate parametrization of the Thomas-Fermi density of neutral atoms.


4:42PM L13.00012 Construction of Wave Function Functionals. MARLINA SLAMET, Sacred Heart University, XIAO-YIN PAN, Ningbo University, VIRAHT SAHNI. The Graduate School, CUNY. — We recently proposed [1] expanding the space of variations in calculations of the energy by considering the approximate wave function \( \Psi = \Phi_0 \) of a function of \( \Phi_0 \), rather than a function. A constrained search is first performed over all functions \( \Phi_0 \) that satisfy a physical constraint or leads to a known value of an observable. A rigorous upper bound to the energy is then obtained via the variational principle. In this paper we apply this idea to the ground state of the He atom by constructing \( \Phi_0 \) that reproduce the exact expectations of the Hermitian single- and two-particle operators \( W = \sum_i r_i^2, n = -2, -1, 1, 2, W = \sum_i \delta(r_i); W_1 = |r_1 - r_2^2|, m = -1, -2, 1, 2 \). The functional \( \Phi_0 \) are of the form \( \Psi_0 = \Phi_0 - f(\chi) \), where \( f(\chi) \) is a prefactor and \( f(\chi) \) a correlation factor. The \( \Psi_0(\chi) \) lead to the exact expectation value of \( W \); (ii) are automatically normalized; and (iii) provide a rigorous upper bound to the energy. [1] X.-Y. Pan, et al, PRA 72, 032505 (2005).

4:54PM L13.00013 LDA+DMFT Charge self-consistency applied to Yb valence transition. ERIK R. YLVISAKER, W. E. PICKETT, UC Davis, A. K. MCMANAHAN, LLNL. — Ytterbium metal, in a pressure range of 0 to 34 GPa, is known to undergo a gradual transition from a \( v^3 f^{14} \) state to a \( v^3 f^{14} \) state where \( v \) and \( f \) represent valence (spd) and d-orbital occupations, respectively. We present, first, conventional LDA+DMFT studies of this transition using both the Hirsch-Fye QMC and Hubbard I atomic solvers. This application of DMFT to the correlated f-orbitals gives reasonable agreement with the experimental transition. However, the neglect of charge self-consistency is questionable for a valence transition where the concentration of valence electrons changes. Therefore we generalize the procedure and compare and contrast LDA+DMFT results (transition pressure, energy and equation of state) with and without charge self-consistency for Yb using the Hubbard I impurity solver.
5:06PM L13.00014 Fock exchange in FLAPW method. TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Fock exchange potential has distinct features which cannot be seen in the LDA exchange potential. (i) It is self-interaction free potential and (ii) nonlocal potential and thus state-dependent potential. With appropriate correlation effects added, these two features may produce significantly improved results over the conventional LDA results, as one can witness in the GW calculations. Massidda et al. (1993) proposed a way to calculate Fock exchange potential of extended solids within the FLAPW method. Their idea was to apply Weinert’s Poisson solver to infinite lattice summation as is done for the Hartree potential calculation. Due to the long range nature of Coulomb interaction, one encounters singularity problem in this process. They handled it by simply extending Gygi’s prescription (1986), which was originally developed for the norm-conserving pseudopotential framework. In this paper, we present our formula in calculating Fock exchange matrix of solids based on the FLAPW method. Following Massidda’s idea, we use Weinert’s Poisson solver. However, in treating the Coulomb singularity, we have developed a more accurate way: the occupied eigenfunctions in Fock operator are expanded up to the second order in terms of \( q \) vector based on the \( k \cdot p \) perturbation theory, whereas Gygi’s way corresponds to the zeroth order expansion. With this higher order expansion, one can achieve faster convergence for the Brillouin zone integration appearing in the Fock operator.

Tuesday, March 11, 2008 2:30PM - 5:30PM —
Session L14 GQI: Focus Session: Foundations of Quantum Theory II Morial Convention Center 205

2:30PM L14.00001 General probabilistic theories for quantum foundations and quantum information. JONATHAN BARRETT, University of Cambridge — Is there any reason why the universe should obey the laws of quantum theory, as opposed to any other possible theory? Is quantum theory special in any way? The best way to address these questions is to view quantum theory as just one point in an entire space of possible theories, and to compare and contrast quantum theory with its rivals. As the success of quantum information theory makes clear, one means by which different theories may be compared and contrasted is via their information processing capabilities. To this end, following early work of Mackey, Ludwig and others, I show how to write down essentially arbitrary probabilistic models, based on the conditions that state spaces are convex and that separated systems cannot be used for instantaneous signalling. Both the classical and quantum theories are special cases. With a focus on information processing, I then describe (i) some features of quantum theory that one might have expected to be uniquely quantum, but turn out to be highly generic, and (ii) some features that do mark quantum theory as special. Some of this is work done in collaboration with Howard Barnum, Matthew Leifer and Alexander Wilce.

3:06PM L14.00002 Fully epistemic toy theory\(^1\), MICHAEL SKOTINIOITIS, AIDAN ROY, BARRY C. SANDERS, Institute for Quantum Information Science, University of Calgary — The Spekkens toy model is an interesting example of how to modify classical physics in order to perform several quantum information processing tasks. Spekkens’ toy model has four axioms concerning toy states, valid operations, measurements, and composition of single toy systems. Motivated by the empirical indistinguishability of epistemic vs. ontic states in the toy universe, we show that relaxing valid operations to mappings of epistemic rather than ontic states preserves the features of the toy model. Similarly we show that relaxing the axiom regarding the composition of single toy systems also preserves the toy model. Relaxing both axioms simultaneously, however, breaks the correspondence of the toy model with quantum theory because the tensor product composition rule is violated, but these two relaxations together produce a group of operations on epistemic states that is isomorphic to the projected extended Clifford Group.

\(^1\) CIFAR, iCORE, NSERC, MITACS

3:18PM L14.00003 Tensor products and teleportation protocols for abstract state spaces. ALEXANDER WILCE, Susquehanna University — In a well-known generalization of classical probability theory, arbitrary compact convex sets serve as abstract “state spaces” for (hypothetical) physical systems, with classical systems corresponding to simplices and quantum systems, to state spaces of \( C^* \)-algebras. One can define natural tensor products for abstract state spaces, modeling composite systems subject to a no-signaling condition. Remarkably, many basic quantum-information-theoretic phenomena, including the no-cloning and no-broadcasting theorems, already appear at this level of generality. However, the existence of a teleportation protocol is a strong constraint, moving us closer to quantum theory. In this talk, after a brief summary of the framework, I will outline what we currently understand about teleportation in this setting. This represents recent and ongoing joint work with Howard Barnum, Jonathan Barrett and Matthew Leifer.

3:30PM L14.00004 The Density Matrix and the Interpretation of Quantum Theory. OWEN MARONEY, Perimeter Institute for Theoretical Physics — Can a density matrix be regarded as a description of the physically real properties of an individual system? If so, it may be possible to attribute the same objective significance to statistical mechanical properties, such as entropy or temperature, as to properties such as mass or energy. Non-linear modifications to unitary evolution can be proposed, based upon this idea, to account for thermodynamic irreversibility. Traditional approaches to interpreting quantum phenomena assume that an individual system is described by a pure state, with density matrices arising only through a statistical mixture or through tracing out entangled degrees of freedom. We discuss how treating the density matrix as fundamental can affect the viability of some of these interpretations, and how the thermodynamically motivated non-linearities do not, in themselves, help in solving the quantum measurement problem.

3:42PM L14.00005 An Approach to Quantum State Pooling from Quantum Conditional Independence\(^1\), MATTHEW LEIFER, University of Waterloo — In approaches to quantum theory in which the quantum state is taken to represent an agent’s belief, knowledge or information about a physical system, it is legitimate for different agents to assign different states to one and the same physical system. The question then arises of what state they should assign if they get together and share their information about the system. This is the problem of quantum state pooling. The classical counterpart of this problem for probability distributions only has a unique solution under additional assumptions about how the data are collected, such as conditional independence constraints. Recently, Spekkens and Wiseman found a quantum pooling rule analogous to the classical one, which is valid if the differing state assignments arise from making indirect measurements on special classes of tripartite quantum state. We show that this pooling rule applies to a much wider class of tripartite states, and that its validity rests on quantum analogs of conditional independence recently studied by one of the authors, as well as a generalization of the notion of a sufficient statistic to the quantum case. Work done in collaboration with Robert Spekkens, University of Cambridge.

\(^1\) ML was supported in part by grant RFP-06-006 from The Foundational Questions Institute (fqxi.org).

4:18PM L14.00006 New results in the category-theoretic approach to foundations of quantum physics. BOB COECKE, Oxford University — We report on some recent results in the category theoretic approach quantum physics, which aims to provide an operational foundation, a logical axiomatics as well as a purely diagrammatic language for it. Firstly, we were able to unify several measurement-based quantum computational schemes; in particular, the categorical language is sufficient to provide proofs of universality for each of these. Secondly, we have a manner to abstractly generate arbitrary multi-partite entangled states; hence equipping multi-partite entanglement with a formal interpretation in terms of information-flow. Also, we axiomatised Spekkens’ model in purely category-theoretic terms; its quantum-like behaviors are now consequences merely of abstract category-theoretic structure.
4:30PM L14.00007 Graphical Calculi and Mutually Unbiased Embeddings of Classical Logic


1This work supported by EPSRC Postdoctoral Research Fellowship EP/E045006/01.

4:42PM L14.00008 Basing quantum theory on information processing

HOWARD BARNUM, Los Alamos National Laboratory — I consider information-based derivations of the quantum formalism, in a framework encompassing quantum and classical theory and a broad spectrum of theories serving as foils to them. The most ambitious hope for such a derivation is a role analogous to Einstein’s development of the dynamics and kinetics of macroscopic bodies, and later of their gravitational interactions, on the basis of simple principles with clear operational meanings and experimental consequences. Short of this, it could still provide a principled understanding of the features of quantum mechanics that account for its greater-than-classical information-processing power, helping guide the search for new quantum algorithms and protocols. I summarize the convex operational framework for theories, and discuss information-processing in theories therein. Results include the fact that information that can be obtained without disturbance is inherently classical, generalized no-cloning and no-broadcasting theorems, exponentially secure bit commitment in all non-classical theories without entanglement, properties of theories that allow teleportation, and properties of theories that allow “remote steering” of ensembles using entanglement. Joint work with collaborators including Jonathan Barrett, Matthew Leifer, Alexander Wilce, Oscar Dahlsten, and Ben Toner.

Supported by the US DOE through the LDRD program at LANL.

5:45PM L14.00009 Quantum mechanics and the nature of the second law of thermodynamics

IAN T. DURHAM, Saint Anselm College — The second law of thermodynamics is inherently a classical law, though quantum analogues have been suggested. What are these quantum analogues and what is their relation to the classical version of the second law? In particular, what can Bell’s inequalities tell us about this relation? This continues ongoing work, some of which has been presented at previous APS meetings, and makes a stronger argument on the thermodynamic nature of Bell’s inequalities.

5:06PM L14.00010 Many worlds and the appearance of probability in quantum mechanics

ROBERT A. VAN WESEP — The theory of measurement has posed a conceptual problem since the beginning of quantum mechanics (QM). On the one hand, the quantum theory of measuring systems says that when a system measures the value of a quantity \( A \) associated with a system \( \mathcal{S} \), the state of the compound system \( \mathcal{S}\mathcal{O} \) following the measurement is a superposition of pure product states, one for each eigenvalue of \( A \). On the other hand, one’s subjective experience (as the observer \( \mathcal{O} \)) is that this statevector “collapses” nondeterministically to a pure state with probability given by the Born rule. The Copenhagen interpretation (CI) says that this collapse actually occurs. The many-worlds view (MW) is that it doesn’t. The defects of CI are obvious: there is no way to say which interactions are measurements to which the interpretation applies, and there is no way to describe the process of collapse that it calls for. MW, on the other hand, does not seem able to incorporate the Born rule. If this were true, it would rule out MW as a description of reality. We show that it is not true, in the strongest possible way: the Born rule is actually a derivable consequence of the quantum theory of measurement as long as we accept the theory as is, i.e., as long as we accept MW[1]. The proof uses the strong law of large numbers, which is the link between the abstract notion of probability and the concrete properties of sequences of observations.


5:18PM L14.00011 Quantum catalysis of information

KOJI AZUMA, Department of Materials Engineering Science, Osaka University, MASATO KOASHI, NOBUYUKI IMOTO, Department of Materials Engineering Science, Osaka University; CREST — In quantum information science, it has been long believed that no one can access quantum information in a system without disturbing it. In fact, the belief has been corroborated by several no-go theorems such as the no-cloning theorem and the no-deleting theorem. Here, however, we show that the belief is incorrect, by exhibiting a novel process, ‘quantum catalysis of information’, in which, without receiving any disturbance, a system certainly exchanges a type of information that cannot be transmitted without quantum communication channel.

Tuesday, March 11, 2008 2:30PM - 5:18PM
Session L15 GQI: Focus Session: Progress toward Scalable Quantum Information Processing
Morial Convention Center 207

2:30PM L15.00001 Ensemble encoding of quantum registers: it’s easy if you can count to one

KLAUS MOLMER, Lundbeck Foundation Theoretical Center for Quantum Systems Research, University of Aarhus — We present a new encoding of qubits in multi-bit registers which makes use of the collective population of a set of internal states of an ensemble of identical quantum systems. This establishes a linear rather than exponential relationship between the number of bits and the internal state Hilbert space dimension of our basic physical system. The key requirement of our proposal is that we can count to one and restrict the collective populations to the values zero and unity. We propose physical implementations and recipes for one- and two-bit gates with ground state atoms interacting via Rydberg excited states, offering up to 14 bits in a small cloud of cesium atoms, and with polar molecules interacting via a stripline cavity field and a Cooper pair box, offering even larger register sizes.

In collaboration with Etienne Brion, Imperial College; Line Hjortshøj Pedersen, University of Aarhus; Mark Saffman, University of Wisconsin; and Karl Tordrup, University of Aarhus.
3:06PM L15.00002 Progress toward scalable optical quantum computing1. PAUL KWIAT, University of Illinois at Urbana-Champaign — Quantum computing holds great promise for solving certain problems which would be intractable using classical computing architectures. Compared to other carriers of other quantum information (e.g., ions, spins, or superconductors) photons have the simultaneous advantage and disadvantage of interacting with the environment and each other only weakly. They are thus relatively immune to decoherence, but it is difficult to achieve the required qubit-qubit interactions. Fortunately, in 2001 Knill, Laflamme, and Milburn proposed a scheme that was scalable at least in principle, if not in practice (too many resources per gate were required). Since then, the ideas were merged with those of “one-way quantum computing” to realize a scalable approach based on “cluster states”, with much more modest though still very challenging – resource requirements. Here I will describe some of the challenges and recent successes, both in implementing the necessary resources (i.e., high-efficiency detectors, single- and entangled-photon sources, and fast logic), and in applying these to realize some basic quantum computing primitives (single- and two-qubit gates and some simple algorithms).

1This work was supported by the IARPA QCCM project “Optical Quantum Computing”

3:42PM L15.00003 Experimental demonstration of decoherence-free one-way quantum information processing, ROBERT PREVEDEL, Faculty of Physics, University of Vienna, MARK S. TAME, The Queen’s University, Belfast, ANDRÉ STEFANOV, IQOOI, Austrian Academy of Science, MAURO PATERNOSTRO, MYUNGSHIK KIM, The Queen’s University, Belfast, ANTON ZEILINGER, Faculty of Physics, University of Vienna and IQOOI, Austrian Academy of Science — In recent years, one-way quantum computing has become an exciting alternative to existing proposals for quantum computers. In this specific model, coherent quantum information processing (QIP) is accomplished via a sequence of single-qubit measurements applied to an entangled resource known as cluster state. However, there has so far been no experimental realization of noise-resilient quantum computation in the one-way model. Here we report the experimental demonstration of a one-way quantum processor reliably operating under the effects of decoherence. Information is protected by a properly designed decoherence-free subspace in which the cluster states reside. We demonstrate our scheme in an all-optical setup by encoding the information into the polarization of states of four photons. A one-way information-transfer protocol is performed with the photons exposed to severe symmetric phase damping noise. Remarkable protection of information is accomplished, delivering nearly ideal computational outcomes.

3:54PM L15.00004 Entangling the optical frequency comb into multiple continuous-variable cluster states1. OLIVIER PFISTER, HUSSAIN ZAIDI, University of Virginia, NICOLAS MENICUCCI, Princeton University and the University of Queensland, STEVEN FLAMMIA, Perimeter Institute for Theoretical Physics, RUSSELL BLOOMER, MATTHEW PYSHER, University of Virginia — A single multimode optical parametric oscillator (OPO) can be designed so that its nonlinear gain medium (typically a two-photon parametric amplifier) generates a particular network of entangling interactions between the eigenmodes of its optical cavity. We show how this can be formulated using nonstandard graph states and how these are related to the usual graph states, an example of which is the cluster state for one-way quantum computing. We also report on the progress of our very compact experimental implementation, in a single OPO with a single pump field, of a parallel quantum register comprising several independent quadripartite cluster states.  

1NCM acknowledges support from the U.S. Dept. of Defense and the National Science Foundation, STF from ONR Grant No. N00014-07-1-0304, and HZ, RB, MP, and OP from NSF Grants No. PHY-0555522 and No. CCF-0622100.

4:06PM L15.00005 Experimental Teleportation-Based Quantum Gate, KAI CHEN, ALEXANDER GOEBEL, CLAUDIA WAGENKNICHT, YU-AO CHEN, JIAN-WEI PAN, PHYSIKALISCHES INSTITUT, RUPRECHT-KARLS-UNIVERSITÄT HEIDELBERG, GERMANY, TEAM, HEFEI NATIONAL LABORATORY FOR PHYSICAL SCIENCES AT MICROSCALE AND DEPARTMENT OF MODERN PHYSICS, USTC TEAM — For large scale quantum computation, the major challenge for entangled qubits is the environment-induced interaction between them. Teleportation-based scheme offers an alternative way for scalable quantum computing. Most attractively, this architecture allows for realizations of universal quantum gates in a fault-tolerant manner as shown by Gottesman and Chuang, and in fact serves as an important basis for measurement-based quantum computing. We report a proof-in-principle experimental implementation of this architecture by demonstrating a teleportation based two-qubit CNOT (controlled NOT) gate through linear optics with 6-photon scheme. By preparation of high-fidelity four-photon cluster states and applying two Bell state measurements with the photons of our very compact experimental implementation, in a single OPO with a single pump field, of a parallel quantum register comprising several independent quadripartite cluster states.

4:18PM L15.00006 Generation arbitrary permutation symmetric state with projection, FANGWEN SUN, Optical Nanostructures Laboratory, Columbia University, New York, NY 10027, CHEE HAE WONG, OPTICAL NANOSTRUCTURES LABORATORY, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 TEAM — We proposed a scheme to generate arbitrary permutation symmetric multi-partite state. The system contains N equally single quantum particles (We use atoms for these particles) which may interact with single photon to generate entanglement between them. This entanglement can be obtained by the transition from three-level \( \lambda \) atom’s exited state to different low levels and emitting corresponding polarized photon, or by inputting a single-photon to a trapped atom to gain different phase shift . After preparing N photon-atom entangled states, the N photons are combined into same path mode to erase the Welcher-Weg information. By postselection \( (N-k) \) photons in one polarization state and \( (N+k) \) photons in its orthogonal polarization state with N-fold coincidence counts, we can generate the atom Dicke state \( \left\{ \frac{N-k}{N+k} \right\} \). Moreover, the arbitrary superposition of these Dicke states can be generated by constructing corresponding projection measurements, which includes multi-atom GHZ state. Based on the discussion on the entanglement between different degrees of freedom, we will show that the projection measurement can also be constructed in the far-field region without combining all photons in one path mode.

4:30PM L15.00007 Single photon Mach-Zehnder interferometer for quantum networks based on the Single Photon Faraday Effect: principle and applications, HUBERT SEIGNEUR, CREOL, University of Central Florida, MICHAEL LEUENBERGER, NanoScience Technology Center and Dept. of Physics, University of Central Florida, WINSTON SCHEFFIELD, CREOL, University of Central Florida — Combining the recent progress in semiconductor nanostructures along with the versatility of photonic crystals in confining and manipulating light, quantum networks allow for the prospect of an integrated and low power quantum technology. Within quantum networks, which consist of a system of waveguides and nanocavities with embedded quantum dots, it has been demonstrated in theory that many-qubit states stored in electron spins could be teleported from one quantum dot to another via a single photon using the Single Photon Faraday Effect. However, in addition to being able to transfer quantum information from one location to another, quantum networks need added functionality such as (1) controlling the flow of the quantum information and (2) performing specific operations on qubits that can be easily integrated. In this paper, we show how in principle a single photon Mach-Zehnder interferometer, which uses the concept of the single photon Faraday Effect to manipulate the geometrical phase of a single photon, can be operated both as a switch to control the flow of quantum information inside the quantum network and as various single qubit quantum gates to perform operations on a single photon. Our proposed Mach-Zehnder interferometer can be fully integrated as part of a quantum network on a chip.
4:42PM L15.00008 High threshold 2D nearest neighbor quantum computation. , AUSTIN FOWLER, PETER GROSZKOWSKI, Institute for Quantum Computing, Waterloo; ROBERT RAUSSENDORF, University of British Columbia — We describe a quantum computation scheme on a 2D nearest neighbor coupled square lattice of qubits that requires relatively few physical qubits per logical qubit, permits logical operations between arbitrarily distant logical qubits in almost constant time and has a physical gate threshold error rate of almost 1%. To the best of our knowledge, no other quantum computation scheme simultaneously possesses all of these desirable properties.

4:54PM L15.00009 A Universal Operator Theoretic Framework for Quantum Fault Tolerance. , GERALD GILBERT, MITRE Quantum Information Science Group; ROBERT CALDERBANK, VANEET AGGARWAL, Princeton University; MICHAEL HAMRICK, YAAKOV WEINSTEIN, MITRE Quantum Information Science Group — We introduce a universal operator theoretic framework for quantum fault tolerance. This incorporates a top-down approach that implements a system-level criterion based on specification of the full system dynamics, applied at every level of error correction concatenation. This leads to more accurate determinations of error thresholds than could previously be obtained. The basis for the approach is the Quantum Computer Condition (QCC), an inequality governing the evolution of a quantum computer. In addition to more accurate determination of error threshold values, we show that the QCC provides a means to systematically determine optimality (or non-optimality) of different choices of error correction coding and error avoidance strategies. This is possible because, as we show, all known coding schemes are actually special cases of the QCC. We demonstrate this by introducing a new, operator theoretic form of entanglement assisted quantum error correction.

5:06PM L15.00010 Structure and quantum-dynamics relationship in spin networks , LUIS CAJAMARCA, LUIS QUIROGA, Universidad de los Andes — We report on the relationship of the spin dynamics with the quantum network topology. The network consists of N-1 spins-1/2 arranged along a circle, also referred to as a ring, equidistant to a central spin (Heisenberg star or ring topology). Every spin along the ring interacts with its first neighbors by means of a constant coupling J1, as well as with the central spin by means of a constant coupling J1. Both couplings are of antiferromagnetic nature and the competition among these incorporates the well known magnetic frustration behavior, which is characteristic of this type of systems. A full analysis of the quantum system's dynamics is carried out for the two limiting cases of coupling constants. We analyze the ground state transitions of the system as well as correlations between any pair of spins including the temperature dependence. The time evolution of the central spin is also analyzed for a given preparation state of the whole spin network. Finally, an stochastic element is incorporated into the system by disconnecting the central spin with any spin along the ring in a random manner. Such dynamics is referred to as dilution and allows us to describe how quantum quantities, such as spin coherences, entanglement and general quantum correlations, depend on the different path topologies between the considered spins (classical structural quantities). Extensions to more complex network topologies are also addressed.

Tuesday, March 11, 2008 2:30PM - 5:30PM –

Session L16 DBP: Focus Session: Brownian Motors Morial Convention Center 208

2:30PM L16.00001 Stochastic path integrals and geometric theory of mesoscopic stochastic pumps and reversible ratchets. , ILYA NEMENMAN, LANL — A variety of stochastic systems, from enzyme kinetics to epidemiology, exhibit pump-like behaviors, where adiabatic changes of parameters result in a nonzero directed current through the system. Using the stochastic path integral technique from mesoscopic physics, we have been able to relate these and similar phenomena to geometric effects in mesoscopic stochastic kinetics and construct their unifying theory. In the talk, this methodology will be demonstrated on three examples: (1) an adiabatic pump effect in the evolution of a Michaelis-Menten enzyme, treated as a classical two-state stochastic system; (2) a reversible ratchet; and (3) a related novel phenomenon in a previously unexplored domain, namely the SIS epidemiological model. In all of these examples, pump-like currents follow from very similar geometric phase contributions to the effective action.

3:06PM L16.00002 ABSTRACTS WITHDRAWN –

3:18PM L16.00003 Failure of Overdamped Models for Buttiker-Landauer Heat Engine: Molecular Dynamics Simulation , RONALD BENJAMIN, RYOICHI KAWAI, University of Alabama at Birmingham — A spatially inhomogeneous temperature profile in presence of a periodic potential leads to directed current of Brownian particles, commonly known as Buttiker-Landauer ratchet. Under a small external load the system can do work as a heat engine. Overdamped models, neglecting inertial effect (m = 0), predict that the engine can reach Carnot efficiency. On the other hand, the overdamped limit (m → 0) predicts the opposite due to the kinetic energy contribution to the heat transfer, suggesting that m = 0 is mathematically a singular point. A phenomenological argument predicts that the heat from the hot to the cold reservoir diverges as 1/√m [1,2]. We confirmed this singular behavior by Molecular Dynamics (MD) simulation and also by numerically solving the corresponding inertial Langevin equation. We obtain good agreement between the MD simulation and the inertial Langevin equation whereas the solution of the overdamped Langevin equation qualitatively disagrees with them. We also confirmed, from the numerical simulation, that the efficiency of the engine does not reach the Carnot limit.


3:30PM L16.00004 Modeling an efficient Brownian heat engine , MESFIN ASFAW TAYE, National Central University Jongli, 32054 Taiwan — We investigate the effect of subdividing the ratchet potential on the performance of a tiny Brownian heat engine that modeled as a Brownian particle hopping in a viscous medium in a sawtooth potential (with or without load) assisted by alternately placed hot and cold heat baths along its path. We obtain analytic expression for the steady state current. The expressions for velocity, efficiency and coefficient of performance of refrigerator are reported for different number of barrier subdivisions. We find that the velocity, the efficiency and the coefficient of performance of the refrigerator maximize as the number of barrier subdivisions increase.

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1Supported by DOE under contract No. DE-AC52-06NA25396

2Supported by MITRE under grant #07MSR205, by the National Science Foundation under grant #1096066 and the Air Force Office of Scientific Research under contract #00852833
3:42PM L16.00005 Trajectories of a Brownian Motor, DEAN ASTUMIAN, University of Maine — Many bio-molecular motors are dimers that move by a “hand-over-hand” mechanism along polar bio-polymeric tracks. Examples include kinesin, that “walks” on microtubule and myosin V that “walks” on actin. These molecular motors share two important symmetries. Typically the motor dimers have approximate mirror symmetry, and their tracks have translational, but not mirror, symmetry. Here we use a trajectory approach to analyze a minimal model for a generic dimeric motor that moves on a polymer track incorporating these two symmetry features. The analysis focuses on the relative probabilities of forward, reverse, backward, backward reverse trajectories and provides an experimentally accessible measure of the relative importance of a “Brownian motor” vs. “Power stroke” mechanism. Reciprocal relations, similar to those derived for the linear regime by Onsager for the fluxes (generalized velocities), hold for arbitrary magnitude forces (i.e., far from the linear regime) for the net probabilities for stepping and for chemical reaction.

4:18PM L16.00006 ABSTRACT WITHDRAWN —

4:30PM L16.00007 Nonequilibrium Fluctuations and Mechanochemical Couplings of a Molecular Motor, ANDY LAU, Florida Atlantic University, DAVID LACOSTE, ESPCI, KIRONE MALICK, CEA Saclay — We investigate theoretically the non-equilibrium features of a single processive motor operating far from equilibrium using an extension of the two-state model introduced by Kafri et al [Biophys. J. 86, 3373 (2004)]. By including an important variable, namely, the number of ATP consumed, we construct a thermodynamic framework, which allows us to characterize the ATP consumption rate of a motor, its run length, and its thermodynamic efficiency. Additionally, with the aid of the Fluctuation Theorem, we analyze the violations of Einstein and Onsager relations as functions of generalized forces. Our main results are (i) one of the Einstein relations holds near stalling, (ii) the degree by which the Onsager symmetry is broken is largely determined by the underlying asymmetry of the substrate, (iii) kinesin’s maximum efficiency and its maximum violation of Onsager symmetry occur roughly at the same energy scale, corresponding to that of an ATP hydrolysis (~ 20 k_BT).

1Support from NSF DMR-0701610

4:42PM L16.00008 Influence of non-conservative optical forces on the dynamics of optically trapped colloidal spheres: The fountain of probability, BO SUN, YOHAI ROICHMAN, ALLAN STOLARSKI, DAVID G. GRIER, Center for Soft Matter Research, New York University — We demonstrate both experimentally and theoretically that a colloidal sphere trapped in an optical tweezer does not come to equilibrium, but rather reaches a steady state in which its probability flux traces out a toroidal vortex. This non-equilibrium behavior can be ascribed to non-conservative optical forces and constitutes a particularly simple thermal ratchet. We briefly discuss ramifications of this effect for previous experiments in which optical tweezers have been treated as conservative potential energy wells.

4:54PM L16.00009 Anomalous single-particle diffusion in a tilted washboard potential, KE XIAO, YAEEL ROICHMAN, Center for Soft Matter Research of New York University, SANGHYUK LEE, University of California, Berkeley, DAVID GRIER, Center for Soft Matter Research of New York University — A corrugated optical vortex acts as a tilted washboard potential for micrometer-scale colloidal particles. A single particle circulating around a corrugated optical vortex undergoes normal diffusion in the limit of strong driving and high temperatures. In the opposite limit, a particle becomes localized. When the effective barrier height is comparable to the thermal energy scale, the particle switches intermittently between stationary and running states. This intermittent switching results in a giant enhancement of the particle’s effective self-diffusion coefficient, which has been predicted theoretically and demonstrated experimentally. The observed enhancement is at least one order of magnitude larger than predicted. Simulations of this system reveal that, contrary to predictions, the single particle undergoes anomalous diffusion, and that this explains the unexpectedly large enhancement of the thermally driven fluctuations. In particular, we show that giant diffusivity arises from the competition between sticking and running states, and can be related to the anomalous diffusion characteristics. We show that the system crosses over from superdiffusive behavior to subdiffusion as the driving increases relative to the barrier height, in agreement with experiments.

5:06PM L16.00010 New Proposed Mechanism for Actin-Polymerization-Mediated Propulsion, KUN-CHUN LEE, ANDREA LIU, University of Pennsylvania, Department of Physics and Astronomy — An important component of the cellular cytoskeleton is F-actin, a biopolymer whose non-equilibrium self-assembly is key to the process of cell crawling. We have reported previously how the polymerization and branching of F-actin near the cell membrane drives cell crawling using a physically-consistent Brownian Dynamics model. Here we show that the creation of new polymerizing filaments by the branching process leads to a steady-state concentration profile of actin away from the moving surface. This non-equilibrium concentration profile is associated with an osmotic pressure profile. The gradient of the osmotic pressure, evaluated at the surface, is the force density on the actin. This force pushes actin backwards, away from the surface. By Newton’s third law, this force has a reaction force on the disk; this is the force pushing the disk forwards.

1This work is supported by NSF-CHE06-13331 and UPenn MRSEC NSF-DMR05-20020.

5:18PM L16.00011 Stochastic Regulation of Actin Bundles Growth Dynamics, PAVEL ZHURAVLEV, YUEHENG LAN, GAREGIN PAPOIAN, Department of Chemistry, The University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290 — Actin polymerization in living cells exemplifies biological dynamical processes where mechanics is intrinsically coupled to chemistry. Modeling the dynamics of biochemical reaction networks may by itself be challenging, because ordinary chemical kinetics is often inapplicable when a small copy number of individual proteins are involved. Instead, to treat large fluctuations, the reaction dynamics should be computed with stochastic methods. We have developed an extensible mechano-chemical model describing the dynamics of actin bundle growth and retraction, where all reaction and diffusion processes are treated stochastically. We have applied our computational algorithm to study the dynamics of filopodia, where polymerization rate at the tip is coupled to the membrane force and fluctuations. Our approach allows to investigate how a particular regulatory protein, participating in the relevant signaling network, influences the distribution of filaments in the bundle, growth and retraction rates and other dynamical characteristics. Among these proteins, the most interesting are capping proteins (that block polymerization), formins (that promote polymerization), fascins (that connect the filaments in the bundle together) and myosins (molecular motors that have been observed in filopodia and may participate in active transport to the tip).
The search for supersolidity was given impetus by recent experiments in which solid helium appeared to decouple from a torsional oscillator, but other phenomena which characterize superflow have not yet been observed. Both experiments and theory indicate that defects are involved in supersolidity and these should also affect the solid’s mechanical behavior. We have measured the shear modulus of solid helium at extremely low frequencies and strains, using a new method, and observe anomalous stiffening at temperatures below 200 mK. It has the same dependence on temperature, measurement amplitude, \(^4\text{He}\) impurity concentration and annealing as the torsional oscillator decoupling. This elastic behavior is explained in terms of a dislocation network which is pinned by \(^3\text{He}\) at the lowest temperatures but becomes mobile above 100 mK. Moving dislocations appear eliminate the decoupling and disrupt possible supersolidity.

This research was supported by grants from NSERC Canada and the University of Alberta.

The shear modulus of solid \(^4\text{He}\) increases substantially in the temperature range below 200 mK where torsional oscillator measurements showed mass decoupling apparently associated with supersolidity. The amount of helium which decoupled depended on the oscillator amplitude, which was interpreted in terms of a supersolid critical velocity of order 10 microns/second. We observed a similar amplitude dependence in our shear modulus anomaly - the stiffening at low temperatures decreased above a critical drive level. By varying the measurement frequency (from 20 to 2000 Hz) and by changing the sample’s dimensions, we conclude that the amplitude dependence we see is a function of the stress or displacement in the solid helium rather than the velocity. This contrasts with recent torsional oscillator measurements in which the amplitude dependence scaled with sample velocity. However, the amplitude dependence in our modulus measurements begins at stresses comparable to those in torsional oscillators and at low temperatures it shows hysteretic behavior similar to that seen in torsional oscillators.

This research was supported by grants from NSERC Canada and the University of Alberta.

The shear modulus of solid \(^4\text{He}\) has been investigated as a function of stress or displacement in the solid helium. If we exclude supersolidity, we find the inferred increase in the shear modulus is necessary to account for typical frequency shifts in TO studies is significantly larger than that reported in Ref. [1] and nearly unphysical. Experiments are in progress to understand the connection between NCRI and the increased shear modulus. [1] J. Day and J. R. Beamish, arXiv:0709.4666v1 (2007).

This work is supported by NSF under grant DMR-0706339.

We have constructed a compound torsional oscillator which could be operated at two resonant modes (the first at 496 and the second at 1172 Hz). This device allowed us to study the non-classical rotation inertia of the identical solid \(^4\text{He}\) at the two oscillator modes driven separately. We present here recent studies of NCRI when the two modes are simultaneously excited. The idea was to drive the first mode at high amplitude and to detect its effect on NCRI fraction by the second mode. We expected that when the solid \(^4\text{He}\) was driven at high amplitudes with the first mode to produce significant reduction in NCRI fraction, the same reduction would be measured with the second mode driven simultaneously at very low amplitude. On the contrary, the observed reduction in NCRI fraction by the second mode was much smaller than that expected from the first mode. If the driver/detector roles of the first and second modes were reversed, the amount of reduction of NCRI fraction detected and induced by a high drive amplitude of the second mode became greater in the first mode driven at a low amplitude. The critical drive amplitude effects of NCRI induced in one mode are not entirely “seen” by the other mode in our oscillator.

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This work is supported by NSF grant DMR-0704120.

Supported address: ISSP, Univ. of Tokyo
3:42PM L17.00007 Torsional oscillator and synchrotron x-ray experiments on solid helium in aerogel, J. WEST, M.H.W. CHAN, Dept. of Physics, the Penn State University, University Park, Pennsylvania 16802, N. MULDERS, Dept. of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, C.N. KODDITUWAKKI, C.L. BURNS, Dept. of Physics, Western Michigan University, Kalamazoo, Michigan 49008, L.B. LURIO, Dept. of Physics, Northern Illinois University, Dekalb, Illinois 60155 — A number of Torsional Oscillator experiments have shown that the Non Classical Rotational Inertia fraction in solid $^4$He is strongly dependent on sample preparation. Samples presumed to be the most pristine show the smallest fraction, rapidly quenched samples a much larger one. On the assumption that samples grown in a strongly disordered environment would similarly show a large NCRIff, we have made T.O. measurements on solid samples grown in 95% porous silica aerogel. Contrary to expectation, these samples show a behavior that is very similar to high purity samples grown from the superfluid phase. Subsequent x-ray diffraction experiments show that the solid grown in aerogel is highly polycrystalline, with a hcp crystal structure (as in bulk) and a crystallite size of approximately 100 nm. X-ray diffraction experiments were performed at the Advanced Photon Source, Argonne national laboratory. This work was supported through NSF DMR-0706339 (MHW) and DE-FG01-05ER05-02 (CAB).

3:54PM L17.00008 Non-classical response of solid helium confined in Vycor glass$^1$, DUK YOUNG KIM, CSQR and Department of Physics, KAIST, R.O.K., HYUNG CHAN KIM, Research and development division,NFRC, R.O.K., EUNSEONG KIM, CSQR and Department of Physics, KAIST, R.O.K., KAIST TEAM, NFRC COLLABORATION — The non-classical rotational inertia of solid $^4$He was observed by a series of torsional oscillator experiments$^1$. Probable heat capacity signature of the supersolid transition which coincides with the non-classical mass decoupling is also observed$^2$. Recent torsional oscillator experiments suggest that disorder and the orientation of a helium crystal may play an important role in the appearance of non-classical rotational inertia. Accordingly, the investigation on the role of defects and crystal orientation may provide crucial clues to understand supersolidity. Solid helium confined in porous media cannot possess well-defined crystal orientation and is likely heavily populated with defects. Here we will present the pressure dependence of the non-classical rotational inertia in solid helium confined in Vycor glass by torsional oscillator techniques. $^1$ E. Kim and M. H. W. Chan, Science 305, 1941 (2004); Nature 425, 227 (2004); J. Low Temp. Phys. 138, 859 (2005); Phys. Rev. Lett. 97, 115302 (2006). $^2$ X. Lin, A. C. Clark, M. H. W. Chan, Nature 449, 1025 (2007).

This work is supported by the Creative Research Initiative program of KOSEF.

4:06PM L17.00009 Torsional oscillators and the entropy dilemma of solid $^4$He, M.J. GRAF, A.V. BALATSKY, I. GRIGORENKO, S.A. TRUGMAN, (LANL), Z. NUSSINOV, (WUSTL) — Solid $^4$He is viewed as a nearly perfect Debye solid. Yet, recent calorimetry measurements by Chan’s group (JLTP 138 (2005) 853 and Nature 449 (2007) 1025) indicate that at low temperatures the specific heat has both cubic and linear contributions. These features appear in the same temperature range where measurements of the torsional oscillator period suggest a supersolid transition. We analyze (Phys. Rev. B 76 (2007) 094501) the heat and compare the measured with the estimated entropy for a proposed supersolid transition with 1% superfluid fraction and find that the observed entropy is too small. We suggest that the low-temperature linear term in the specific heat is due to a glassy state that develops below such a mixture of tunneling systems in the crystal. We propose that dislocation related defects produce those tunneling systems. Further, we argue (Phys. Rev. B 76 (2007) 014530) that the reported mass decoupling is consistent with an increase in the oscillator frequency as expected for a glass-like transition. The glass model offers an alternate interpretation of the torsional oscillator experiments in contrast to the supersolid nonclassical rotational inertia (NCRI) scenario.

4:18PM L17.00010 The excitation spectrum of solid $^4$He$^1$, JOHN GOODKIND, University of California, San Diego, ELIZABETH BLACKBURN, SUNIL SINHA, COLLIN BROHOLM, JOHN COPLEY — Speculation about a possible Bose condensation in solid $^4$He has existed for decades and has recently been further stimulated by the discovery of an acoustic anomaly and a decrease in the moment of inertia at temperatures below 200 mK. The excitation spectrum played an important role in understanding the properties of superfluid liquid helium so that, if there is such a condensation in solid $^4$He, the spectrum might also confirm it and aid in understanding it. We have measured the excitation spectrum of solid $^4$He by neutron scattering using the Disc Chopper Spectrometer at NIST. We have identified a sharp line in the spectrum as vacancy wave excitations. The dispersion relation for these excitations has a minimum energy of 1 meV and is quadratic. This vacancy mode intersects the longitudinal phonon mode at 1.1 meV and the two become degenerate at higher energies. The degenerate mode has a linear dispersion law with smaller slope than the longitudinal acoustic mode at lower energies. No change in the spectrum was observed below 200 mK. The spectrum has strong similarities to the spectrum in superfluid liquid helium.

1 work supported by the NSF.

4:30PM L17.00011 Torsion Oscillator Studies of Solid Helium-4$^1$, ETHAN PRATT, BENJAMIN HUNT, Cornell University, MINORU YAMASHITA, Cornell University and Kyoto University, J.C. SEAMUS DAVIS, Cornell University — We will present results of torsion oscillator experiments on solid helium-4 below 300 mK.

This work was supported NSF grant 0434801.

4:42PM L17.00012 Pairing states for the ring exchange t-J model, MING LOU, MICHAEL MA, University of Cincinnati, FU-CHUN ZHANG, University of Hong Kong — Multiple spin interactions, introduced by ring exchange process, are important for many systems, including solid $^3$He and High Tc cuprates. In high Tc cuprates, the dominant term is the 2-spin antiferromagnetic interaction, which leads to d-wave singlet pairing upon doping. In solid $^3$He, on the other hand, the 4-spin interaction plays an important role, and it’s interesting to determine how the Cooper pairing state may differs from that of cuprates. In this work, we apply the renormalized mean-field theory$^1$ to a modified t-J model, where the J term includes the 4-spin interaction introduced by the ring exchange. Our result shows that a mixed state of singlet and triplet pairing optimizes the energy. At half filling, the pairing state is unphysical, due to the fact that there is no double occupancy. Upon doping or with intrinsic vacancies, the paring state becomes physical. Such a mechanism may introduce supersolidity in bulk solid $^3$He and solid $^3$He absorbed on a substrate at very low temperature. $^1$ F.C. Zhang, C. Gros, T.M. Rice and H. Shiba, Supercond. Sci. Technol. 1 36 (1988).

Tuesday, March 11, 2008 2:30PM - 5:42PM
Session L18 DPOLY: Focus Session: John H. Dillon Medal Symposium
Morial Convention Center 210

2:30PM L18.00001 John H. Dillon Medal Talk: Polymer Droplets, KARI DALNOKI-VERESS, McMaster University — The simplicity of a liquid droplet, say a dew drop on spider silk, is both esthetically beautiful and scientifically intriguing. The interplay of surface energies, thermal motion, and confinement of the liquid, especially on small length scales can reveal interesting physics. Droplets are an ideal confining geometry because the length scales can be easily controlled and it is possible to arrange the system such that each droplet acts as an independent experiment. The talk will focus on some recent examples where we have used the droplet geometry to learn about material properties. It will become apparent in the presentation that the deviations from the "expected" behaviour in confined systems are far from subtle!
Lett. 71, 938 (2005)). Our results allow to understand the large deviation from the Manning law observed in these experiments.

Our predictions are in very good agreement with the recent experimental measurements of the effective charge by Essafi et al. (Europhys. Lett. 70, 938). This allows us to calculate the effective electric charge of the pearl as a function of the structure reminiscent of the Rayleigh instability of a charged droplet. Using a Poisson-Boltzmann approach, we calculate the counterion distribution around a given pearl assuming the latter to be penetrable for the counterions. This allows us to calculate the effective electric charge of the pearl as a function of the structure reminiscent of the Rayleigh instability of a charged droplet.

3:30PM L18.00004 Comparison of surface mobility of polymeric and low molecular weight glass-formers. MARK EDIGER, STEPHEN SWALLEN, KEN KEARNS, University of Wisconsin-Madison — The last ten years has seen considerable effort to understand dynamics at the surface of polymer melts and glasses. For comparison, we present data on two low molecular weight glass formers: trisnaphthylbenzene (TNB) and indomethacin (IMC). Neutron reflectivity provides direct information about mobility in the top several nanometers of TNB glasses. Two other measurements (surface crystal growth rates and the enthalpy of glasses prepared by vapor deposition) offer indirect information on surface mobility for IMC and TNB. These measurements indicate that surface dynamics at Tg are 2-5 orders of magnitude faster than bulk dynamics. The temperature dependence of the surface relaxation process is weak below the bulk Tg, in qualitative agreement with recent measurements on polymer surfaces in this regime.

4:2PM L18.00005 Modeling Solvent Evaporation from Glass-Forming Polymer Films by MD Simulations, JORG BASCHNAGEL, SIMONE PETER, HENDRIK MEYER, Institut Charles Sadron, Strasbourg — By means of molecular-dynamics simulations we study solvent evaporation from glass-forming, free-standing and supported polymer films. Polymers are represented by a commonly employed bead-spring model, solvent molecules are modeled as Lennard-Jones particles, and polymer-solvent interactions are tuned such that good-solvent conditions are realized. We start the simulations from a dense solution with a solvent content of 20% and explore the evaporation process for temperatures T above and below the glass transition temperature Tg of the pure polymer film. At all T we observe the formation of a polymer-rich crust at the free surface upon solvent evaporation. For T > Tg we can reproduce the simulation results (reduction of film thickness with time, solvent and polymer density profiles, etc.) by a Fickian diffusion model with a constant diffusion coefficient. For T < Tg deviations from Fickian diffusion are observed. We suggest that these deviations may be rationalized by a diffusion coefficient of the solvent, which depends on film composition and distance from the free surface. We attempt to compare our results to recent experiments.

5:4PM L18.00006 Studies of Glassy Colloidal Systems Under Shear, MICHAEL MASSA, CHANJOONG KIM, DAVID WEITZ, HSEAAS, Harvard University — In analogy with the glass transition of polymer (and other molecular) liquids, colloidal suspensions can undergo dynamic arrest to form a glassy state, when the system is concentrated beyond a critical volume fraction. However, in contrast to their molecular counterparts, studies of the glass transition in colloidal systems are facilitated by their natural length- and time-scales, which make it possible to directly visualize the behavoir of the individual constituent particles. Using confocal microscopy, we follow the dynamics of colloidal suspensions near the glass transition, and in particular, their reaction to an imposed deformation. We investigate the evolution from a quiescent solid to a shear melted liquid, to elucidate the nature of the structural rearrangements that govern the properties of glassy materials.

6:06PM L18.00007 Growth and Stability of Polymer Surface Wrinkles, ALFRED CROSBY, University of Massachusetts — For certain materials and geometries, the surface of a polymer film will wrinkle upon the application of a critical in-plane stress due to surface tension. The resulting morphology minimizes the in-plane strains and the system energy by locally bending the surface plane. This process and morphology have been studied at an increasing rate over the last decade and demonstrated in applications ranging from materials metrology to adhesion control. In general, the knowledge and use of this phenomenon has been developed for conditions that far exceed the point of initiation, under static equilibrium. In this presentation, we highlight recent experiments that explore the growth and morphological transitions of surface wrinkles. We quantify the growth mechanism under different conditions of mechanical constraint and demonstrate a unique ability to stabilize a wide variety of unique, non-predicted, surface wrinkle morphologies.

4:18PM L18.00008 Toughening Mechanisms in Polymer Gels, HUGH BROWN, University of Wollongong — I will describe a simple model that accounts for the very high toughness of double network gels. The model is based on the assumption that the first, stiff network will break up forming multiple cracks when the stress is above a defined value. These cracks are held together by the second network. A multiply cracked damage zone will form round any macroscopic crack in the material causing energy dissipation and shielding the second network. The toughness enhancement by this process is estimated to be about x40. Other techniques of gel toughening will then be discussed.

4:30PM L18.00009 Theory of polymer crystallization, M. MUTHUKUMAR, UMMASS, Amherst — We will present new conceptual arguments for the spontaneous selection of very small lamellar thicknesses and their melting behavior.

4:42PM L18.00010 On the effective charge of hydrophobic polyelectrolytes, ELIE RAPHAEL, UMR CNRS Gulliver 7083, ESPCI, 10 rue Vauquelin, 75005 Paris, France, ALEXEI CHEPELIANSKII, Laboratoire de Physique des Solides, UMR CNRS, 8502, Bat. 510, Universite Paris-Sud, 91405 Orsay, France, FARSHID MOHAMMAD-RAFIEE, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45195, P.O. Box 45195-1159, Iran — In this paper we analyze the behavior of hydrophobic polyelectrolytes. It has been proposed that this system adopts a pearl-necklace structure reminiscent of the Rayleigh instability of a charged droplet. Using a Poisson-Boltzmann approach, we calculate the counterion distribution around a given pearl assuming the latter to be penetrable for the counterions. This allows us to calculate the effective electric charge of the pearl as a function of the chemical charge. Our predictions are in very good agreement with the recent experimental measurements of the effective charge by Essafi et al. (Europhys. Lett. 71, 938 (2005)). Our results allow to understand the large deviation from the Manning law observed in these experiments.
4:54PM L18.00011 Disentanglement in thin polymer films, HENDRIK MEYER, ULP Institut Charles Sadron, CNRS UPR22, Strasbourg, France — Molecular dynamics simulations of thin polymer films confined between structureless walls show accelerated in-plane dynamics with decreasing film thickness. Using the primitive path analysis (PPA) introduced by Everaers et al. [Science 303 (2004) 823] for chain length up to N = 1024, we can show that the entanglement density decreases with decreasing film thickness. However, the effect becomes pronounced only for films thinner than the bulk radius of gyration where also the chain structure becomes modified by the confinement [1]. The PPA algorithm can be modified to estimate the contribution of self-entanglements. The latter become more important for thinner films, however, they do not counterbalance the global decrease of entanglements. [1] H. Meyer et al. Eur. Phys. J. Sp.Top. 141 (2007) 167.

5:06PM L18.00012 Complex Structural Packing of ABC Triblock Copolymers Solvent Annealed at High Humidity, CHUANBING TANG, University of California Santa Barbara, JOONA BANG, Korea University, GILA STEIN, GLENN FREDICKSON, CRAIG HAWKER, EDWARD KRAMER, University of California Santa Barbara, MICHAEL SPRUNG, JIN WANG, Argonne National Laboratory — The use of ABC triblock copolymers to obtain industrially relevant morphologies for block copolymer lithography has been investigated. Nanoporous thin films of poly(ethylene oxide)-poly(methyl methacrylate)-polystyrene triblock copolymer spheres were prepared by solvent annealing under controlled humidity followed by UV degradation and acid washing. Ordered half spheres at the surface that template ordering of spheres below the surface in thin films were formed as a result of the interaction between the highly hydrophilic PEO segments and water vapor in the chamber. The spherical block copolymer domains exhibit complex packing behavior on the surface and in the interior which is dependent on film thickness. Half sphere “monolayer” and half sphere plus whole sphere “bilayer” formed in thin films were shown to have hexagonal lattice symmetry. For half sphere plus two whole sphere “trilayers”, the coexistence of regions of hexagonal and square packing was observed by TEM, SFM, SEM and GISAXS. Square packing was consistent with a surface truncated unit cell of a body-centered cubic lattice with the (100) plane parallel to the surface.

5:18PM L18.00013 High resolution structure of bacterial cell sacculi, JOHN DUTCHER, AHMED TOUHAMI, VALERIO MATIAS, ANTHONY CLARKE, University of Guelph, MANFRED JERICHO, Dalhousie University, TERRY BEVERIDGE, University of Guelph — The major structural component of bacterial cell walls is the peptidoglycan sacculus, which is one of nature’s strongest and largest macromolecules that allows the cell to maintain a large internal pressure while allowing the transport of molecules into and out of the cell and cell growth. The three-dimensional structure of this unique biopolymer is controversial, and two models have been proposed: the planar model, in which the glycan strands lie in the plane of the cell surface, and the scaffold model, in which the glycan strands lie perpendicular to the cell surface. In this study we have used atomic force microscopy (AFM) to investigate the high resolution structure of isolated, intact sacculi of both Gram-positive and Gram-negative bacterial cells. We have observed a sponge-like structure for both types of sacculi with pore diameters between 5 to 15 nm. Our data for Gram-positive sacculi provide evidence for the validity of the scaffold model, whereas our data for Gram-negative sacculi indicate an orientation along the short axis of the cell which is consistent with the planar model. To further elucidate the structure, we have exposed sacculi to the tAmiB enzyme which cleaves peptide-peptide bonds.

5:30PM L18.00014 Mechanical Response of Lipid Multilayers From Micro- and Nanoparticle Embedment, GREGORY MCKENNA, Texas Tech University, KIRTHI DESHPANDE, Texas Tech University — We have used atomic force microscopy (AFM) to image micro- to nano-meter sized particles embedded into lipid multilayer films prepared by a spin coating technique. The lipid investigated was 1,2-dipalmitoyl-Sn-glycerol-3-phosphotidylcholine (DPPC). Gold, silica and polystyrene were used for the embedding particles. Particle diameters ranged from 50 to 300 nm and all tests were performed at atmospheric conditions and ambient temperature. Film thickness was approximately 87 nm based on AFM determination. We used the elastic analysis for contact between a rigid sphere and elastic substrate with the work of adhesion wA acting as the force on the sphere to determine the shear modulus G in terms of wA, the particle radius and the height of the sphere that remains above the surface. From the AFM height measurements, we find that the shear modulus for the DPPC falls in the range from 3 to 30 MPa, but seems independent of particle type and particle size. The potential for the particle embedment method for mechanical property determination of soft materials will be discussed.

This work is partially supported by the National Science Foundation under Grant CMII-0559596.

Tuesday, March 11, 2008 2:30PM - 5:06PM — Session L19 DMP: Focus Session: Dopants and Defects in Semiconductors II, Morial Convention Center 211

2:30PM L19.00001 Highly Enriched 28Si – A New Testbed for Impurity and Defect Structure, MIKE THEWALT, Simon Fraser University — We have recently found that many optical transitions in Si, including those of shallow impurity bound excitons, and the electronic ground state to excited state transitions of shallow donors and acceptors, are remarkably sharper in highly enriched 28 Si than in natural Si, due to the removal of inhomogeneous isotope broadening. This work is now being extended to deeper defects, many of which have been studied for decades. We will show that high resolution spectroscopy in highly enriched Si exhibits transitions which are sharper than in natural Si by a factor of 10. Isotopic substitutions for hydrogen and nitrogen result in the expected frequency shifts, thereby providing an unambiguous identification of these complexes. The N-H stretches are stable up to ~700 °C. The introduction of neutral N-H complexes could prove useful in achieving reliable p-type conductivity in ZnO.

This work was supported by the National Science Foundation (DMR-0704163).

3:06PM L19.00002 Nitrogen-hydrogen complexes in ZnO: A possible route toward p-type conductivity, M.D. MCCLUSKEY, Washington State University, S.J. JOKELA, University of Georgia — Zinc oxide (ZnO) is a wide band gap II-VI semiconductor with optical, electrical, and mechanical applications. The lack of reliable p-type doping, however, has prevented it from competing with other semiconductors such as GaN. In this talk, I describe the successful incorporation of nitrogen-hydrogen (N-H) complexes in ZnO during chemical vapor transport (CVD) growth, using ammonia as an ambient. The N-H bond-stretching mode gives rise to an infrared (IR) absorption peak at 3150 ± 6 cm⁻¹. Isotopic substitutions for hydrogen and nitrogen result in the expected frequency shifts, thereby providing an unambiguous identification of these complexes. The N-H complexes are stable up to ~700 °C. The introduction of neutral N-H complexes could prove useful in achieving reliable p-type conductivity in ZnO.
3:18PM L19.00003 Vibrational lifetimes of O-H stretch modes in MgO and ZnO, ERIK SPAHR, GUNTER LUPKE, College of William and Mary, NORMAN TOLK, Vanderbilt University, LEONARD FELDMAN, Rutgers University — Hydrogen is an important and omnipresent impurity in a wide class of oxides. A more complete understanding of the role of hydrogen in wide-bandgap oxides such as MgO and ZnO is crucial for further development of oxide-based optoelectronics. We have measured for the first time the vibrational lifetime of the O-H stretch mode associated with the Mg$^{2+}$ vacancy in MgO for the charge state, $V_{OH}^-$, and the neutral state, $V_{OH}^0$, using picosecond transient bleaching spectroscopy. For the $V_{OH}$ center we find the lifetime (~11 ps) is longer than for the charged defect state (~5 ps). These lifetimes are almost an order of magnitude shorter than in ionic semiconductors Si and Ge [1].

3:30PM L19.00004 Carrier Dynamics and Photoexcited Emission Efficiency of ZnO:Zn Phosphor Powders, JOHN V. FOREMAN, HENRY O. EVERITT, Dept. of Physics, Duke University, Durham, NC 27708 and U.S. Army Aviation and Missile RDEC, Redstone Arsenal, AL 35898, JIE LIU, Dept. of Chemistry, Duke University, Durham, NC 27708 — The undoped and Ga-doped ZnO thin films were grown on sapphire using molecular-beam epitaxy (MBE) system. The samples of electron concentrations ranging from $1.4 \times 10^{19}$ to $3.4 \times 10^{19}$ cm$^{-3}$ were grown and studied. The RT PL peaks show a monoton red shift from 3.280 to 3.229 eV with the increase of electron concentration, which is attributed to the band-gap narrowing effect. The red-shifted peak values have been fitted. The evolution of the LT PL spectra were studied and discussed. The free exciton emission at 3.371 eV, the first Ga-level-related peak at 3.313-3.321 eV, and the second Ga-level-related peak at 3.359 eV (assigned as the Ga $D^X$ peak) are competing with each other in the LT PL spectra. These three kinds of peaks are dominating in the lightly (or undoped), mediate, and heavily doped ZnO:Ga samples, respectively. From the experiments, we conclude that there are two Ga levels in ZnO. In the lightly doped sample, the Ga atoms contribute to the first Ga level around 3.352 eV. When the Ga incorporation reaches some critical amount, Ga atoms form the second Ga level in ZnO at 3.359 eV.

3:42PM L19.00005 Study of the carrier concentration dependent photoluminescence of Ga-doped ZnO thin films grown by molecular-beam epitaxy, ZHENGYANG, LEELAPRASANNA MANDALAPU, JILIN LIU, Quantum Structures Laboratory, Dept. of Electrical Engineering, University of California, Riverside — The undoped and Ga-doped ZnO thin films were grown using molecular-beam epitaxy (MBE) system. The samples of electron concentrations ranging from $1.4 \times 10^{19}$ to $3.4 \times 10^{19}$ cm$^{-3}$ were grown and studied. The free exciton emission at 3.371 eV, the first Ga-level-related peak at 3.313-3.321 eV, and the second Ga-level-related peak at 3.359 eV (assigned as the Ga $D^X$ peak) are competing with each other in the LT PL spectra. These three kinds of peaks are dominating in the lightly (or undoped), mediate, and heavily doped ZnO:Ga samples, respectively. From the experiments, we conclude that there are two Ga levels in ZnO. In the lightly doped sample, the Ga atoms contribute to the first Ga level around 3.352 eV. When the Ga incorporation reaches some critical amount, Ga atoms form the second Ga level in ZnO at 3.359 eV.

3:54PM L19.00006 Zinc Vacancy induced magnetism in ZnO thin films and nanowires, QIAN WANG, Virginia Commonwealth University, QIANG SUN, Peking University, PURU JENA, Virginia Commonwealth University — Extensive theoretical studies based on first-principles have been carried out for the mechanism of magnetism in ZnO thin films and nanowires. It has been identified that the observed magnetism is introduced by Zn vacancy and is affected by its concentration. The main source of the magnetic moment comes from the unpaired 2p$^-$ electrons in oxygen sites around the Zn vacancy, instead of Zn 3d electrons. Moreover, Zn vacancy is more energetically favorable to reside on the surface, and its formation energy is found to be less than that of oxygen vacancy that does not introduce any magnetism. These findings suggest that the main vacancy species is Zn vacancy as expected by experiments. The present theoretical study not only provides some deep understandings for the experimentally observed magnetism in un-doped ZnO samples, but also suggests that introducing Zn vacancy is a natural and an effective way to fabricate magnetic ZnO structure for bio-magnetic applications.

4:06PM L19.00007 Magnetism of Undoped and Co-Doped TiO$_2$ Clusters, X. WEI, R. SKOMSKI, M. SCHUBERT, D. SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska — TiO$_2$ is a widely used optically active material, and transition-metal doped TiO$_2$ has attracted much attention in spintronics. Recently, it has been argued that ferromagnetism is a universal feature of nanoparticles of nonmagnetic oxides, and our focus is on doped and undoped TiO$_2$ nanoclusters. The clusters are examined with TEM, AFM, MFM, and hysteresis loops and zero field cooled magnetization curves were measured by SQUID magnetometry. Both doped and undoped films display hysteresis and magnetic order in the investigated temperature range of 50K to 400K. The ordering temperature is above 400 K, and both magnetization and coercivity are enhanced in the out-of-plane direction. Undoped TiO$_2$ particles exhibit a nominal moment of about 0.2 $\mu_B$ per surface atom. Small Co concentrations have little effect on the magnetism of the particles. Higher Co doping percentages, about 5%, yield prototropic (clockwise) loops, indicating the formation of CoO. It has been suggested that the magnetic moment of 'nonmagnetic' oxide thin films is a surface effect, and the comparison of different particle sizes yields a similar picture for our particles. Our renormalization-group modeling assumes indirect exchange interactions between scarce magnetic moments and yields a logarithmic dependence of the ordering temperature on the particle size - This research is supported by NSF MRSEC and NCMN.

4:18PM L19.00008 First-principles determination of the electronic structure of native point defects and impurities in rutile TiO$_2$. JUN HE, Argonne National Laboratory, SUSAN SINNOTT, University of Florida — Density-functional theory calculations are used to determine the electronic structures of native point defects (Ti interstitials and O vacancies) and dopants (Al and Nb) in rutile TiO$_2$. The calculated densities of states (DOS) show that in pristine and defective structures that contain charged Ti interstitials or O vacancies, the lower conduction bands of the defective structures are shifted up in energy relative to the perfect structure. This shift leads to a broader lower conduction band that more readily promotes the formation of shallow donor levels. This effect is more pronounced in the case of Ti interstitials. We also find that the charge state of the Ti interstitial influences the extent of orbital overlap. The case of Al dopants is much more complex since Al can either be a donor or an acceptor. In the case of Al and Nb substitutional defects, the calculated DOS is similar to the DOS of the pristine structure.

1This work is supported by the National Science Foundation (DMR-0303279)

4:30PM L19.00009 Group III-A Acceptor-Hydrogen interactions in SnO$_2$, JOEL VARLEY, Physics Department, University of California, Santa Barbara, CA 93106, ANDERSON JANOTTI, ABHISHEK SINGH, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106 — Using first-principles calculations we investigate the role of hydrogen in the passivation of p-type dopants in SnO$_2$. We focus on group III-A elements, including Al, Ga, and In and investigate the stability of these impurities when substituting Sn under hydrogen-free and hydrogen-rich conditions. Hydrogen effectively passivates the acceptors and removes their electrical activity. Based on calculated binding and migration energies we discuss conditions under which hydrogen can be removed and acceptor activation can take place. We also calculate the stretch-mode vibrational frequencies associated with the hydrogen-impurity complexes, providing a signature for experimental identification in vibrational spectroscopy. We conclude that the group III-A elements studied are suitably shallow acceptors for p-type doping and that the presence of interstitial H will not impede, and potentially enhance, p-type doping of SnO$_2$. 

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4:42PM L19.00010 Investigation of Electroluminescent Degradation in doped ZnS phosphors1, FRANK BRIDGES, JACOB STANLEY, YU JIANG, LAUREL RUHLEN, JOHN WILLY, SUE CARTER, Physics Dept. UCSC Santa Cruz 95064 — We present optical and EXAFS data on a series of ZnS samples doped with Cu, Mn and Cl. These materials (30 micron particles) have a strong electroluminescence (EL) when subjected to a 100V square-wave voltage. At 100 Hz, the luminescence decays significantly in a 20 hr period. We show that this degradation can partially be reversed by annealing the sample and that this can be repeated several times. In addition the EL emission centers reoccur at the same points in the 30 micron particles after the anneal. The optimum annealing temperature is about 180°C, but varies slightly for different wavelengths. Surprisingly an anneal at somewhat higher temperatures (240°C) dramatically reduces the EL intensity. The EXAFS studies show that the local structure about Cu continues to look like Cu2 for “as made”, EL degraded, rejuvenated samples (annealing at 180°C), and thermally degraded samples (annealed at 240°C). This means that most of the Cu is in the relatively inert CuS precipitates, and does not change significantly with EL degradation or annealing. Thus the EL active sites must be dilute. We discuss some possible models.

1Supported by DOE Grant DE-FG02-07ER46388

4:54PM L19.00011 Theoretical Study of native defects in CdGeAs2, TULA R PAUDEL, Department of Physics, Case Western Reserve University, WALTER R.L. LAMBRECHT, Department of Physics Case Western Reserve University — First-principles results are presented for various native defects viz. : V_{Cu}, V_{Ge}, V_{As}, Cd_{As}, Ge_{Cd}, Ge_{As}, Ge_{As}, and As_{Cd}, in CdGeAs2 under different growth conditions. The defects were calculated by constructing a 64 atom supercell in the full potential linearized muffin-tin orbital implementation of the density functional theory under the local density approximation (LDA). Calculations of the energy of formation show that antisites should be the most abundant type of defect. The LDA band gap is adjusted to experimental band gap by introducing a non-local orbital dependent constant potential shift to the s-orbitals of Cd and Ge and d-orbitals of Cd within the LSDA+U approach. The defect transition levels for different charge states are calculated. The calculations support the earlier suggestion that Ge_{As} is a shallow acceptor. The calculated transition levels are found to be significantly different form corresponding defects levels of ZnGeP2. The defect levels are interpreted in a simple molecular-orbital theory and compared with the available experimental data.

Supported by AFOSR

Tuesday, March 11, 2008 2:30PM - 5:30PM
Session L20 DMP: Focus Session: Self-Assembled Organic Overlayers Morial Convention Center 212

2:30PM L20.00001 Self-assembly at the liquid/solid interface: from patterns to function, STEVEN DE FEYTER, K.U.Leuven — Self-assembly - the spontaneous organization of molecules into stable, structurally well-defined aggregates - has been put forward as a possible paradigm for generating nanoscale templates under ambient conditions. A very convenient method for the formation of extended two-dimensional (2D) networks is physisorption at the liquid-solid interface. The preparation is relatively simple and scanning tunneling microscopy (STM) allows a detailed investigation of the structural aspects of the 2D patterns. A deep understanding and control of the spatial orientation and packing of molecules in self-assembled systems is indispensable for the development of future nanodevices. We have developed hydrophobic - hydrophilic nanopatterns at electirfied surfaces via the self-assembly of amphiphilic molecules. For this purpose we selected 5-hexadecyloxysphotic acid: this neutral amphiphile forms hydrogen-bonded rows that are commensurate with the Au(111) surface. Based on the successful adsorption of these amphiphiles, multicomponent architectures have been realized at these electirfied surfaces as the result of the potential directed assembly of charged and non-charged molecular systems. Following a slightly different approach, nanoporous two-dimensional networks were formed at the interface between an organic liquid and highly oriented pyrolytic graphite. Pore sizes of more than 5 nm in diameter can be realized. As an alternative approach to make nanoporous two-dimensional networks, molecular defined shape-persistent two-dimensional oligomers, such as molecular spiked wheels, are used.

3:06PM L20.00002 Stress-Induced Striped Domains at the C60-Pentacene Interface*, DANIEL DOUGHERTY, National Institute of Standards and Technology, WEI JIN, Department of Chemistry and Biochemistry and Materials Research Science and Engineering Center University of Maryland at College Park, WILLIAM CULLEN, Department of Physics and Materials Research Science and Engineering Center University of Maryland at College Park, GREGORY DUTTON, JANICE REUTT-ROBEY, Department of Chemistry and Biochemistry and Materials Research Science and Engineering Center University of Maryland at College Park, STEVEN ROBEY, National Institute of Standards and Technology — Cd60:pentacene heterojunctions have been recently employed in functional organic photovoltaic devices [1]. In order to develop a detailed structural understanding of these junctions, we have made STM observations of the growth of pentacene on top of a monolayer film of C60 on Ag(111). We observe pattern formation in the first pentacene layer due to the tensile stress arising from interactions with the underlying C60. The stress results in a striped pattern of alternating commensurate and incommensurate domains of pentacene with respect to the C60 monolayer. The incommensurate domains appear as bright regions 3.6 ± 0.6 nm in width and are discussed using a 1D Frenkel-Kontorova model. *Supported by the NIST Center of Nanomanufacturing and Metrology and the University of Maryland MRSEC via DMR-05-20471 [1] Yoo et al., Appl. Phys. Lett. 85, 5472 (2004).

3:18PM L20.00003 The growth mechanism of Pentacene-C60 heteroepitaxial films, A. AL-MABBOO, J.T. SADOWSKI, Y. FUJIKAWA, T. SAKURALI, Institute for Materials Research, Tohoku University — Pentacene (Pn) and fullerene (C60) are of great interest among organic semiconductors as they show highest field-effect hole and electron mobilities respectively. The absorption peak in Pn crystal is located close to maximum of solar visible spectra, making a bipolar Pn-C60 diode promising for solar cell application. In order to improve its efficiency to satisfy the requirement for practical application, an in-depth understanding of Pn-C60 interface formation is necessary for further optimization. We shall discuss the growth mechanism of Pn-C60 heteroepitaxial films on Bi(0001)/Si(111) substrate studied by real time low-energy electron microscopy and complementary scanning tunneling microscopy. A competitive growth between a thin-film phase of Pn having standing-up orientation and a phase with laying-down orientation has been observed. The growth of laying-down phase is suppressed gradually with increasing film thickness. The nucleation of this phase is also suppressed with increasing temperature and the standing up phase without co-presence of laying down phase is achievable at ~75°C.

3:30PM L20.00004 Self-Limiting C60-Pentacene Network on Ag(111)1, WEI JIN, University of Maryland, DANIEL DOUGHERTY, National Institute of Standards & Technology, GREGORY DUTTON, WILLIAM CULLEN, University of Maryland, STEVEN ROBEY, National Institute of Standards & Technology, JANICE REUTT-ROBEY, University of Maryland — During Scanning Tunneling Microscopy investigations of C60:Pentacene (Pc) interfaces on Ag(111), we identified a new network structure. This binary arrangement forms readily by sequential deposition: Pc, of 0.3 mL coverage, is first evaporated onto the Ag(111), forming a 2-D grid. Subsequent C60 deposition produces a network, consisting of chains of close-packed C60 molecules, spaced by C60 molecules. The characteristic 1 x 2.5 nm2 pores are sized to accommodate Pc molecules. Spontaneous formation of this structure from an initial Pc coverage ranging from 0.6 to 0.6 mL, indicates a self-limiting assembly process. Drawing upon topographic and Z(V) measurements, we propose a structural model and describe molecular mechanisms that could cause this self-limiting behavior.

1Supported by the Dept. of Commerce through the NIST Center of Nanomanufacturing and Metrology and the NSF-funded MRSEC via DMR-05-20471.
3:42PM L20.00005 Guest-host interaction of C_{60} adsorbed on an ordered layer of phthalocyanine derivatives, TOMAS SAMUELY, MEIKE STOEHR, NIKOLAI WINTJES, University of Basel (Switzerland), THOMAS A. JUNG, Paul Scherrer Institute (Switzerland), MARCO HAAS, SHI-XIA LIU, SILVIO DECURTINS, University of Bern (Switzerland) — Symmetrically substituted phthalocyanines (Pcs) with eight peripheral di-(tert-butyl)phenoxy (DTPO) groups self-organize on noble metal substrates. The rotational degrees of freedom, specific for the DTPO substituents, allow a bowl-like conformation of the Pc derivatives and thus, hosting of the C_{60} molecules in two clearly distinguishable binding sites. Moreover, controlled manipulation of the C_{60} by the STP enables switching from one site to the other. Since Pcs are well-known electron donors and C_{60} molecules are good acceptors, it can be conceived as a system with two morphologically different donor-acceptor complexes, individually addressable by an STP tip. Preliminary STS analysis shows vast differences in the electronic properties. Exploration of such a system is of great interest because of its similarity to fundamental biological processes (photosynthesis, respiration), as well as its potential application in energy storage, conversion, nanoelectronics, etc.

3:54PM L20.00006 Scanning Tunneling Microscopy Investigation of Ordered Iron Phthalocyanine Molecules on Ag(111), KEN PARK, KEDAR MANANDHAR, Baylor University, S. MA, JAN HRBEK, Brookhaven National Laboratory — A well-ordered, molecular thin films (about 0.5 monolayers) of iron phthalocyanine (FePc) on Ag(111) has been investigated using a scanning tunneling microscopy. The room temperature deposition, followed by 30 minutes annealing up to 475 K results in well-ordered islands of FePc molecules which form a two-dimensional, oblique lattice. The overlay lattice vectors a, and b, are 16.2 Å each with the angle of 80° between the lattice vectors. The FePc overlay lattice is commensurate to the substrate lattice with the relationship of a = 6a - b and b, = a + 6b, with a and b, are the Ag(111) lattice vectors. Furthermore, FePc molecules at the opposite corners within the unit cell align their isodole rings at each other, significantly increasing the nearest and the next-nearest neighbor distances in the overlay. The commensurate overlay lattice structure and the distinct molecular orientation within the unit cell are attributed to the molecule-surface interaction via the Fe 3d_{x^2−y^2} and Ag 4d_{x^2−y^2} orbitals.

4:06PM L20.00007 Self-assembly of functionalized fullerenes on strained metallic interfaces, BOGDAN DIACONESCU, MIKAEL JAZDZYK, GLEN MILLER, KARSTEN POHL, University of New Hampshire — The process of growing ordered arrays of molecules or nanometer sized clusters with tailorable properties on the dislocation networks of strained metallic thin films requires a detailed understanding of the nucleation processes and film-molecule and intermolecular interactions. We compare two different self-assembly mechanisms of functionalized fullerenes on strained metal films of Ag on Ru(0001). We found that by controlling the molecular coverage and/or the strain in the thin film, various interactions can dominate the self-assembly process, thus resulting in a richness of structures with controllable properties. At low molecular coverage on 1 monolayer Ag films on Ru(0001), ordered triangular arrays of clusters, 4.9 nm apart, with a tunable number of molecules can be grown. This process is driven by strain relaxation in the metal film, as confirmed by 2D Frenkel-Kontorova models, and was found to be a general one working for various functionalized molecules. At higher molecular coverage and different Ag film thickness, the intermolecular interaction becomes dominant and the symmetry and unit cell size of the self-assembled monolayer are a consequence of the molecular structure and functionality. Both these processes are generally applicable to many functionalized C_{60} molecules thus opening avenues towards complex self-organized structures based on lock and key type approach.

4:18PM L20.00008 Morphology of thin organic semiconductor layers on vicinal (0001) sapphire surface, GVIDIO BRATINA, PRIMOŽ REBERNIK RIBIC, University of Nova Gorica — Morphology of pentacene, 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDTA), rubrene, and N,N′-diphenyl-N,N′-bis(3-methylphenyl)-1,1′-diphenyl-4,4′-diamine (TIPD) layers grown on vicinal (0001) sapphire surface was examined by non-contact atomic force microscopy ex situ. The layer thickness ranged from a submonolayer coverage to up to four molecular layers. Pentacene molecules on the terraces in a layer-plus-island growth mode. PTCDTA nucleates randomly at room temperature, while at 135°C and low coverage the molecules aggregate at the steps. At increased coverage the island growth proceeds in the directions determined by the intermolecular interactions and not along the steps. Rubrene and TIPD nucleate in 3D islands that evolve over time by ripening. TIPD nucleates along the steps and also ripening proceeds along the steps. The rate of ripening of rubrene islands is one order of magnitude slower than the rate of ripening of TPD. We associate this difference to the wealth of rotational degrees of freedom in TPD molecules as opposed to only twisting degree of the tetracene backbone in rubrene.

4:30PM L20.00009 Organic Vapor-Liquid-Solid Deposition for Controlled Growth of Organic Semiconductor Films, DAVID PATRICK, BRAD JOHNSON, Western Washington University — Thin films of low molecular weight organic semiconductors (OS) are drawing much attention for their potential use in a range of different applications. Because the optical and electronic properties of OS films are extremely sensitive to structural imperfections, domain size, and crystallographic orientation, preparation of high quality thin films with controlled microstructure under technologically favorable conditions has long been a bottleneck toward practical applications and better controlled fundamental studies. Here we describe an approach for fabricating OS films that comes close to achieving these demanding objectives. The main advance is the combined use of atmospheric pressure chemical vapor deposition (APCVD) and capillary liquid injection (LC) solvent, which is applied as a thin coating onto a supporting substrate, providing an organized fluid environment in which OS crystals nucleate and grow. The technique produces relatively large crystals, enables control over crystallographic orientation, growth habit, and size, and involves near ambient conditions compatible with a variety of substrates and inexpensive processing conditions. Results will be presented for the model compounds tetracene and pentacene.

4:42PM L20.00010 Structure and adsorption mechanisms of thiol self-assembled monolayers on GaAs (001) surfaces, OLEKSANDR VOZNYY, JAN J. DUBOWSKI, University of Sherbrooke — Self-assembly of organic molecules on solid substrates attracts a lot of interest from both fundamental and practical perspectives. Particularly, alkanethiol SAMs on GaAs surfaces can be used, e.g., for surface passivation, bio- and chemical sensing, molecular electronics and nanolithography. However, the progress of the investigation of this material system is hindered by problems of reproducibility of SAMs growth due to insufficient understanding of the deposition process on the atomic level and a lack of experimental characterization techniques. In this work, we present the results of ab initio modeling of thiol SAMs on GaAs (001) surface which helps to resolve the SAM structure, chemistry of bonding to substrate, adsorption kinetics and energetics. We also compare the GaAs case to a prototypical system of thiols on Au and discuss differences the semiconductor surface brings to the process.

4:54PM L20.00011 Self-assembly of long chain alkane and their derivatives on graphite, YANG YANG, SAVAS BERBER, DAVID TOMÁNEK, Michigan State University, JUN-FU LIU, GLEN P. MILLER, University of New Hampshire — We combine scanning tunneling microscopy (STM) measurements with ab initio calculations to study the self-assembly of long chain alkane and related alcohol and carboxylic acid molecules on graphite. For each system, we identify the optimum adsorption geometry and explain the energetic origin of the domain formation observed in the STM images. Our results for the hierarchy of adsorbate-adsorbate and adsorbate-substrate interactions provide a quantitative basis to understand the ordering of long chain alkane in self-assembled monolayers and ways to modify it using alcohol and acid functional groups. Supported by NSF NIRT grant ECS-0506309 and NSF NSEC grant EEC-425826.
5:06PM L20.00012 Theoretical Modelling of Self-Assembly of Molecular Networks, MANUEL MURA, NATALIA MARTSINOVICH, LEV KANTOROVICH, King's College — The phenomenon of self-assembly of atomic and molecular superstructures on crystal surfaces has attracted an increasing interest in nanotechnology. Self-organised nano-templates where the self-assembled monolayer traps other molecules with selected functional properties, can be used as building blocks for larger nanoscale structures. These superstructures can form chiral domains ranging from 1D chains to 2D monolayers. In particular, there have been many scanning tunneling microscopy (STM) studies of self-assembly of melanine, perylene tetra-carboxylic di-imide (PTCDI) or perylene tetra-carboxylic di-anhydride (PTCDA) molecules on the Au(111). STM images of these networks do not reveal the exact details of the intermolecular bonding and process of network growth. It is therefore the task of theory to determine the exact atomic structure of these networks. We present a theoretical study of self-assembly of molecular networks on different molecules by using a systematic approach to build molecular superstructures. The energies of these structures are calculated using the density-functional theory SIESTA code. The theoretically predicted monolayer structures are in very good agreement with the results of STM measurements.

5:18PM L20.00013 Polymerization of a perylene derivative on a metal surface, MANFRED MATENA, JORGE LOBO-CHECA, MEIKE STOEHR, University of Basel, Switzerland, KATHRIN MUELLER, THOMAS A. JUNG, Paul-Scherrer-Institute, Switzerland, TILL RIEHM, LUTZ H. GADE, University of Heidelberg, Germany — By utilizing the concepts of supramolecular chemistry, impressive results for molecular self-assembly on surfaces have been achieved. Mostly, non-covalent interactions like metal coordination, hydrogen bonding or dipolar coupling are exploited to create supramolecular patterns. One approach to influence these structures relies mainly on the sophisticated design of the molecular functional groups. Thus it makes use of properties already inherent to the molecules. In our work we have chosen a different concept. A thermally-induced surface-assisted reaction was used to modify the endgroups of a perylene derivative (TAPP) and thereby, the molecular interactions are altered. TAPP was found to form a closed-packed assembly on Cu(111), whereas the molecular interactions are based upon vdW-forces. After annealing at 150 °C, a rectangular network is obtained which is commensurate to the underlying Cu surface. In this case the organic molecules coordinate to Cu atoms through the lone pairs of their nitrogen atoms.

Tuesday, March 11, 2008 2:30PM - 4:30PM — Session L21 DCP: Focus Session: Clusters, Cluster Assemblies, Nanoscale Materials V Morial Convention Center 213

2:30PM L21.00001 Ab Initio Simulations of Nano-Diamond Surface Reconstruction, WILLIAM MATTSON, RADHAKRISHNAN BALU, US Army Research Laboratory — We have simulated with in the Density Functional Theory (DFT) spherically cut nano-diamonds from bulk diamond at ambient conditions. The 2.6 nanometer diameter sphere is then allowed to relax at 250K and surface reconstruction is observed. Four hemispherical fullerene like regions form on the surface and while the interior maintains the diamond structure, it undergoes compression equivalent to over 30GPa in the bulk. Results of dynamic shearing will be presented.

2:42PM L21.00002 TiO₂ nanocrystals prepared by ferrocene/cobalt catalyst agents¹, M.E. GOMÉZ, J.C. CAICEDO, G. ZAMBRANO, Thin Film Group, Department of Physics, Universidad del Valle, A. A. 25360 Cali, Colombia, A.M. LAZAR, D. CHAUMONT, LRRS and FR 2604 Université de Bourgogne 21078 Dijon, France, Y. LACROUTE, M. SACILOTTI, CMN and LPUB. UFR Sc. Techn. FR 2604 Université de Bourgogne, 9 avenue A. Savary, BP 47870, 21078 Dijon Cedex, France — We present the growth and characterization of TiO₂ nanocrystals. Nanostructured growth is obtained in a low-pressure CVD system by using an organometallic precursor Ti(OCH₃)₄ as both the Ti and O source catalyzed by both ferrocene (an organometallic precursor) and cobalt metallic clusters prepared by the microwave-assisted polyol method. Two kinds of TiO₂ structures were obtained in the cobalt clusters: a) pine-tree like (with short-leaf structure) and b) long-leaf structures as large as a few micrometers in size and both under 10-nm in thickness. Long-leaf TiO₂ structures were grown at cobalt grain boundaries. For the growth conditions utilized, the TiO₂ structures are composed of both anatase and rutile crystallographic phases.

¹This work was accomplished under contract project title FILIMON35 n ANR-05-NANO-016-03 France, and the Excellence Center for Novel Materials - CENM contract 043-2005 with COLCIENCIAS, Colombia.

2:54PM L21.00003 Metal cluster anions produced by attachment of slow electrons: Evaporative cooling, cluster energetics, and restructuring of the abundance spectra¹, VITALY KRESIN, ROMAN RABINOVITCH, CHUNLEI XIA, University of Southern California — Metal clusters are able to attach low-energy electrons with very large cross sections by capturing them in a strong long-range polarization potential. But little information has been available about the last stage of the collision process: what happens to the energy deposited by the captured electron, and are the cluster size distributions modified? We have carried out measurements of the mass spectra of negative sodium cluster ions born in the electron-cluster interaction region. Importantly, the arrangement allowed us to monitor the parent and the daughter cluster beams simultaneously. It is found that the electron affinity energy is quickly thermalized and is sufficient to cause rapid evaporative cooling. As a result, the magic numbers shift from Naₙ to Naₙ⁻. And a host of other significant changes in the abundance structure are observed, compared to the parent cluster beam. These are well reproduced by a detailed analysis based on the evaporation cascade model, and yield new information about cluster binding energies.

¹Supported by NSF

3:06PM L21.00004 Anion Photoelectron Spectroscopy and Density Functional Investigation of Diniobium-Carbon Clusters¹, P.A. CLAYBORNE, Virginia Commonwealth University, K.L. KNAPPENBERGER, JR., University of California, Berkeley and Lawrence Berkeley National Laboratory, J.U. REVELES, Virginia Commonwealth University, M.A. SOBHY, C.E. JONES, JR., U.U. GUPTA, I. IORDANOV, J. SOFO, A.W. CASTLEMAN, JR., Pennsylvania State University, S.N. KHANNA, Virginia Commonwealth University — Experimental photoelectron and computational results show diniobium-carbon (Nb₂C₄) clusters to coexist in multiple structural isomers: three-dimensional geometries, planar rings and linear chains. Three-dimensional clusters having up to five carbons are formed preferentially with Nb-Nb bonding, whereas only Nb-C bonding is observed experimentally at six carbons. Clusters consisting of an odd number of atoms are also observed with linear geometries. The larger binary clusters (n ≥ 7) display properties similar to pure carbon clusters. We provide evidence for niobium substitution of carbon atoms.

¹The authors gratefully acknowledge support from the US Air Force Office of Scientific Research, Grant FA9550-04-1-0066 and FA9550-05-1-0186 and from the Department of the Army through MURI Grant # W911NF-06-1-0280.
3:18PM L21.00005 Towards Artificial Molecules: Metallodielectric Clusters. VINOTHAN MANOHARAN, JONATHAN FAN, Harvard University, SEAS — Recent advances in the synthesis of metallic colloids have allowed for an explosion in research into their optical properties. It is now possible to synthesize solid metallic colloids, core-shell colloids that mix different metals, and core shell colloids of metallodielectrics. In this talk I propose a mechanism for further exploring the optical properties of such materials by producing clusters of metallodielectric colloids and studying the relationship between the structure and composition of a colloidal cluster and its optical response. To this end, we synthesized a number of solutions, each of clusters consisting of a different average number of colloids. By doing this, we hope to study the effects of different dielectrics and near neighbor interactions on the plasmonic resonances of the metallic shells in the colloid. In the future, we hope to produce and study high yield, pure samples, both in solution and as photonic crystals. All of these options provide new ways of producing specific optical resonances that can be used in sensors, spectroscopy, optical triggers, and many other applications.

3:30PM L21.00006 Quantum transport in molecular electronic devices described with complex source and sink potentials. ALFARO, MARTIN JUAREZ FLORES, ANDREAS KOSTER, CINVESTAV, Departamento de Quimica, MARCELA BELTRAN, UNAM, J. ULISES REVELES, GWINN, DIRK BOUWMEESTER, DEBORAH FYGENSON, University of California Santa Barbara — We synthesize fluorescent clusters of silver atoms on metallodielectric colloids and studying the relationship between the structure and composition of a colloidal cluster and its optical response. To this end, we synthesized a number of solutions, each of clusters consisting of a different average number of colloids. By doing this, we hope to study the effects of different dielectrics and near neighbor interactions on the plasmonic resonances of the metallic shells in the colloid. In the future, we hope to produce and study high yield, pure samples, both in solution and as photonic crystals. All of these options provide new ways of producing specific optical resonances that can be used in sensors, spectroscopy, optical triggers, and many other applications.

3:42PM L21.00007 Charge carrier solvation on a polymer chain revealed in ab initio computations. MICHAEL MAYO, YURI GARTSTEIN, The University of Texas at Dallas, Richardson, Texas, USA — When an excess charge carrier (electron or hole) is added to a semiconducting polymer chain in vacuum, it is well known that the carrier may self-trap into a polaronic state accompanied by a self-consistent localized bond alternation pattern. A different mechanism of self-localization is a solvation of the charge carrier expected to take place when the polymer chain is immersed in a polar medium (such as a common solvent) - in this case a self-consistent pattern of the orientational polarization is formed around a localized charge. The goal of our study is to identify this solvation effect within ab initio computations. Using long carbon atom chains (both hydrogen terminated and rings) as model systems, we employ the hybrid B3LYP density functional within the DFT and the Polarizable Continuum Model to find the resulting electronic level structure and atomic charge densities. Our results clearly show trends towards excess charge self-localization due to the solvation. We suggest that this effect may be of importance for various semiconductor nanostructures in polar environments.

3:54PM L21.00008 Nanotubes in polar environments: Solvated charge carriers and their dynamics. GREGORY USSERT, YURI GARTSTEIN, Dept. of Physics, Univ. of Texas at Dallas, Richardson, TX, USA — Excess charge carriers on semiconducting nanotubes immersed in sluggish polar environments (such as common solvents) can undergo self-localization into polaronic states whose properties are profoundly different from the free band states. We explore such solvated states within the adiabatic continuum framework using a simplified picture of an electron or a hole confined to a cylindrical surface in the 3D polar medium. At the static level, the binding energy of a polaron is evaluated and found to be a sizable fraction (~0.3) of the corresponding Wannier-Mott exciton binding energy, which is expected to substantially decrease the thermal activation energy for the exciton dissociation. We discuss the diffusion and mobility of polarons caused by the dielectric fluctuations of the medium and applied electric fields, as well as the local dielectric relaxation modes in the vicinity of the polaron. We also discuss the electronic (optical) transitions between the localized electronic states within a self-consistent potential well due to the orientational polarization pattern.

4:06PM L21.00009 Fluorescent silver atom clusters in DNA hairpin loops. PATRICK O’NEILL, ELISABETH GWINN, DIRK BOUWMEESTER, DEBORAH FYGENSON, University of California Santa Barbara — We synthesize fluorescent clusters of silver atoms on DNA hairpins, and systematically vary the loop region to examine the effects of DNA sequence and structure on the optical properties and chemical stability of the Ag clusters. We find that these novel fluorophores only form on the single stranded hairpin loop, have Stoke’s shifts ranging from 60nm to 120nm and can be tuned to emit at wavelengths ranging from 525nm to 670nm. Furthermore, certain DNA geometries support strong excitation of visible fluorescence by the Ag clusters. We find that these novel fluorophores only form on the single stranded hairpin loop, have Stoke’s shifts ranging from 60nm to 120nm and can be tuned to emit at wavelengths ranging from 525nm to 670nm. Furthermore, certain DNA geometries support strong excitation of visible fluorescence by the Ag clusters.

Tuesday, March 11, 2008 2:30PM - 5:30PM — Session L22 DPOLY: Confinement-Induced Structures in Block Copolymers Morial Convention Center 214

2:30PM L22.00001 Dillon Symposium Break —
curvature influences the defect density in the formed structure.

In particular, the distribution of characteristic morphologies and structure dimensions for a given fiber diameter are characterized. Key novel aspects of this work include sampling of thermal fluctuations in full three dimension, rather than finding minimum energy surfaces and extensive comparison to experimental data on electrospun block copolymer–polymer fibers. Two methodological innovations are also introduced. First, an unprecedentedly precise estimate of Flory $\chi$ parameters for the model allows a quantitative comparison to field theoretic models. Second, a novel reflective boundary model allows common boundary artifacts in total density to be effectively eliminated, even for fibers with of dimensions comparable to single chains.

Complex Morphologies of Symmetric Diblock Copolymers under Nano-Confinement

By employing a bond fluctuation lattice Monte Carlo simulation, block copolymers confined in nano-cylindrical cavities are studied. The effects of preference of the surface for segments and incompatibility between different blocks as well as the symmetry of the chains and the ratio of cavity diameters to the lamellae period of copolymers in the bulk $(D/L_0)$ are investigated in detail. Numerous novel morphologies such as complicated helical structures, plate morphologies with fins and dendrites etc are presented in this work. Some phase diagrams regarding above parameters are provided in order to understand the transitions between structures. Additionally, the orientation parameters indicating the alignments of the polymer chains were calculated and correlated with the morphologies. The simulation results are compared with experimental results qualitatively.

Morphologies of a diblock copolymer melt confined in a spherical nanopore

We systematically investigate the microdomain morphologies that self-assemble in a diblock copolymer melt confined in a spherical nanopore, using real-space self-consistent mean-field theory. Near the surface of the nanopore we find that perforated-layer structures form, with four-, five-, and six-fold coordinated pores, for melts that form the cylindrical phase in the bulk. Simultaneously, spherical domains, toroidal domains, or small networks form in the centre of the pore. We vary the diameter of the pore and accurately locate the diameters where phase transitions between these morphologies occur. The effect of confinement on melts that form spherical microdomains in the bulk is also examined. We find that convergence to regular structures is complicated by the formation of defects, and we develop techniques to eliminate these defects. Methods to distinguish the various morphologies will also be discussed.

Spherical nano-shells of block copolymers

We study the self-assembled morphologies of symmetric diblock copolymers under planner and cylindrical confinement by homogeneous surface(s). The SCF equations are solved with high accuracy in real space, without a priori knowledge of the possible morphologies. Effects of surface preference and film thickness / pore diameter are investigated in detail. In addition to simple morphologies (i.e., surface parallel and perpendicular lamellae), complex morphologies are found in both cases and their stable regions are determined. Our SCF calculations also reveal the formation mechanism of these complex morphologies.

Water permeable nanotubes from amphiphilic block copolymers

By employing a bond fluctuation lattice Monte Carlo simulation, block copolymers confined in nano-cylindrical cavities are studied. The effects of preference of the surface for segments and incompatibility between different blocks as well as the symmetry of the chains and the ratio of cavity diameters to the lamellae period of copolymers in the bulk $(D/L_0)$ are investigated in detail. Numerous novel morphologies such as complicated helical structures, plate morphologies with fins and dendrites etc are presented in this work. Some phase diagrams regarding above parameters are provided in order to understand the transitions between structures. Additionally, the orientation parameters indicating the alignments of the polymer chains were calculated and correlated with the morphologies. The simulation results are compared with experimental results qualitatively.

Effect of curvature on equilibrium and non-equilibrium properties of a 2D smectic phase

We study the Otha-Kawasaki model for diblock copolymers equilibrium and non-equilibrium features of two dimensional smectic phases on curved sinusoidal substrates. At low curvatures defect free patterns are found to be stable. In agreement with theoretical predictions of Vitelli and Nelson [], at high curvatures topological defects are observed in the ground state. In this regime positive (negative) disclinations are located in regions of positive (negative) curvature. The configurations formed by stripes aligned with the lines of longitude are found to be unstable, while the equilibrium state is formed by the stripes aligned with the parallels. General features of smectic phases on curved backgrounds are discussed by a Frank elastic free energy in the one constant approximation.

Phase Transitions in block copolymers under external electric field and in confinements

We describe dynamics of phase transitions of various block copolymer morphologies (lamellae, hexagonally packed cylinders, spheres, gyroid, hexagonally perforated lamellae) under an applied electric field. Second example illustrates kinetics of surface phase transitions in confined systems (thin films).
5:06PM L22.00012 Crystalline Dichloblock Copolymers of Linear Polyethylene - Hydrogenated Polynorbornene, RICHARD REGISTER, SASHA MYERS, SHENG LI, Princeton University — The melt and solid-state morphologies of linear polyethylene (LPE) - hydrogenated polynorbornene (hPN) dichloblock copolymers, and their crystallization behavior, were explored over a range of block ratios and diblock molecular weights. LPE and hPN are both highly-crystalline polymers, with similar melting points, so the final structure can potentially be dictated by the melt structure, or by crystallization of either block. For diblocks with molecular weights of 50 kg/mol, symmetric copolymers exhibited lamellar microphase-separated melts, while diblocks with 20 or 80% LPE were homogeneous, indicating a modest LPE-hPN interaction energy density of approximately 1 J/cc. For the relatively slow crystallizations which can be conducted isothermally, hPN appears to always crystallize first; the two crystallization processes can be resolved by time-resolved DSC and x-ray diffraction at small undercoolings. However, the LPE block has a stronger temperature dependence of its crystallization rate, implying that LPE would crystallize first at deep undercoolings. Up to the highest diblock molecular weights explored (100 kg/mol), crystallization “breaks out” from the melt mesophase to form spherulites defined by the hPN block; subsequent crystallization of the LPE within these spherulites is apparent from a change in optical texture.

5:18PM L22.00013 Deformation-induced structure changes in olefin block copolymer, FENG ZUO, YIMIN MAO, JONGKAH KHEUM, CHRISTIAN EGGGER, BENJAMIN HSIAO, Stony Brook University, HONGYU CHEN, DEBIE CHIU, SHIH-YAW LAI, The Dow Chemical Company — Uniaxial tensile deformation was applied on two olefin block copolymer (OBC) samples to investigate the structure, morphology and orientation development using in-situ small-angle X-ray scattering and wide-angle X-ray diffraction techniques. Two samples have similar molecular characteristics but different chain architectures due to the different content of chain shuttling agent in production. The samples behave alike at room temperature, but the difference becomes distinct at high temperatures, such as fracture strain and crystal orientation. As more chain shuttling agents was used, the more frequently the growing chains transferred between catalysts; shorter block segments are formed. The OBC sample with a 40/60 block ratio has a film thickness of approximately 100 nm. The BCP self assembles into a variety of ordered structures with a period of 100 nm domains. The BCP self assembles into a variety of ordered structures with a period of 200 nm in thickness confining a block copolymer (BCP) to ~100 nm domains. The BCP self assembles into a variety of ordered structures with a period of ~200 nm. A lamellar-in-lamellar structure was achieved and by varying the BCP structure more complex cylinder-in-lamellar and sphere-in-lamellar structures are envisioned. The HP and BCP phase separation/crystallization dichotomy during the formation of hierarchical dielectric mirrors will be discussed.

Tuesday, March 11, 2008 2:30PM - 5:18PM — Session L23 DMP: Focus Session: Probing and Modifying Materials with Lasers II Morial Convention Center 215

2:30PM L23.00001 Femtosecond laser structuring in dielectrics, Saulius Juodkazis, RIES, Hokkaido Univ. — Three-dimensional (3D) structuring of glasses, crystals, and polymers by tightly focused femtosecond laser pulses is a promising technique for microfluidic, micro-optical, photonic crystal and micro-mechanical applications [1-4]. The 3D laser micro-structuring of resists is demonstrated by direct laser writing [1] and holographic recording using phase control of interfering pulses [2]. Tightly focused laser pulses can reach dielectric breakdown irradiance without self-focusing when sub-1 ps pulses are used for laser-structuring inside dielectrics. The limiting case of microstructuring, a void recording, can be achieved [3]. The mechanism of void formation has been explained as a result of dielectric breakdown and micro-explosion. The absorption is localized within a skin depth of tens-of-nanometers in the plasma at the focus. This defines an ultimate localization of the energy delivery by a laser pulse. The absorbance reaches 0.6 in a fully ionized solid state density breakdown plasma. The high temperature and pressure buildup is large enough to generate a shock wave (strong micro-explosion). For example, a single 100 nJ laser pulse forms a void under tight focusing conditions even in the high strength sapphire (Young modulus of 400 GPa). It is considered that material fails upon compression rather than tension for which the mechanical failure threshold is by an order of magnitude smaller. This scenario of breakdown by compression is corroborated by numerical modeling of the strong explosion at our experimental conditions. Modification of materials by tightly focused femtosecond pulses opens new material processing routes for inert dielectrics [4] and can possibly be used for creation of novel high-temperature and pressure phases inside the volume of irradiated samples. These regions with altered nano-structure have different chemical properties as was found in silica glass, quartz, and sapphire by wet etching of the “shocked” regions in aqueous solution of hydrofluoric acid. Current challenges of structural characterization of micrometer-sized volumes of nano-structures materials are discussed. The achievable resolution limits and potential of the fabricated 3D patterns in photonics, micro-fluidics, and sensor applications will be presented. [1] K. K. Seet et al., Adv. Mat. 17, 541, 2005. [2] T. Kondo, et al., New J. Phys. 8, 250, 2006. [3] S. Juodkazis, et al., Phys. Rev. Lett. 96 166101 2006. [4] S. Juodkazis, et al., Adv. Mater. 18 1361 2006.

3:06PM L23.00002 Mechanisms of nanoparticles size reduction by laser irradiation, ALEXANDER Pyatenko, MUNEHIRO Yamaguchi, Masaaki Suzuki, AIST — Size reduction of nanoparticles after laser irradiation is well known phenomenon. Two different mechanisms of size reduction have been proposed: 1) the photoionization of electrons from a particle into a solution which caused ionization and Coulomb explosion of the ionized particle. 2) a simple heating-melting-evaporation mechanism. In this report we show that the different mechanisms are working under different experimental conditions, and give the criterion for their applicability. The main experimental parameter responsible for such criterion is the laser energy flow density, \( I_0 = E/\tau \), where \( E \) and \( \tau \) are the laser pulse energy and duration, and \( S \) is the laser beam cross section. We calculated the critical value for this parameter in case of spherical silver and gold particles. When this parameter exceeds the value of about 10^{10} W/cm^2, the electron ejection can be started. For nanosecond lasers such energy flow density values can be achieved only with beam focusing, but for pico and especially femto lasers this condition can be realized in different experimental arrangements. When \( I_0 \) is smaller than the critical value, the particle heating-melting-evaporation mechanism is responsible for particle size reduction.
3:18PM L23.00003 Novel Nanostructured Materials and Properties by Pulsed Laser Deposition, JAGDISH NARAYAN, COPINATH TRICHI, North Carolina State University — Pulsed laser deposition has been used to create novel nanostructured materials either as layered or nanodot structure. By controlling thin-film growth kinetics during island growth, we are able to create three-dimensional self-assembled nanodot structures of Ni and ordered L10 FePt in a given matrix. Epitaxial growth and Integration of Ni and FePt on Si(100) substrate was achieved via domain matching epitaxy which facilitated epitaxial growth across the misfit scale. Magnetic properties can be varied by controlling the orientation and coercivity higher than 1.2 Tesla achieved. These results on ordered L10 FePt will be compared with those Ni with practical implications of information storage (1,2). (1) H. Zhou, D. Kumar, A. Krots, A. Tiwari, J. Narayan, J. Appl. Phys. 94, 4841 (2003). (2) G.R. Trickey, D. Chakrabarti, J. Narayan, J. T. Prater, J. Phys. D: Appl. Phys 40, 7273 (2007).

3:30PM L23.00004 A study of photoemission using CW and pulsed UV light sources to probe surface slip band structure evolution of single crystal aluminum1, MINGDONG CAI, University of Houston, STEPHEN LANGFORD, J. THOMAS DICKINSON, Washington State University — We report measurements of photoelectron emission from high-purity single crystal aluminum during uniaxial tensile deformation. A 248 nm pulsed excimer laser was used as a light source and the generated photoemission data was compared with that using a filtered mercury lamp. Time-of-flight curves of photoelectrons generated by pulsed excimer laser irradiation were observed showing a two peaked structure. These two peaks correspond to photoelectrons of two energy levels. It was also found that real time total photoelectron charge increases linearly with strain; and the increment is heterogeneous. Photoemission using low-energy photons is sensitive to changes in surface morphology accompanying deformation, including slip line and band formation. The discontinuity in photoelectron intensity and the heterogeneous surface slip band structure prove the production of fresh surface area is not continuous, which is predicted by a recent dislocation dynamics theory based on percolation process. Except for differences in instrumentation and data analysis, the photoemission data from a filtered mercury lamp and from the excimer laser are comparable. Current studies extend the application of the excimer laser into surface dynamics analysis.1 This work was supported by the Department of Energy under Grant DE-FG03-02ER45088.

3:42PM L23.00005 Self-Positioning Optically Trapped Microspheres For Nanoscale Laser Direct Write, CRAIG ARNOLD, EUAN MCLEOD, Princeton University — We present a novel method of near-field laser direct-write patterning by incorporating self-positioning optical manipulation of polystyrene microsphere combined with pulsed laser processing. A 532 or 1064 nm CW laser optically traps a water-dispersed microsphere against a polymer substrate using a 2-dimensional Bessel beam trap. The optical scattering force due to the Bessel beam in the propagation direction is balanced by the repulsive interaction near the surface thereby creating an equilibrium spacing between the two, regardless of large scale surface features. A pulsed nanosecond 355 nm laser directed down the same beam path, is then used to ablate or modify the surface below the microsphere. While the pulsed laser has a large spot diameter, the intensity required for material modification is only achieved directly below the sphere due to focusing and near-field enhancement. Using an x-y translation stage, we demonstrate the ability to move the substrate while keeping the bead fixed in the optical trap, but allowing it to maintain its position above the surface. Direct-write nanoscale features are thereby enabled through this process. Characterization of the resulting structures along with advantages and limitations of this technique will be discussed.

3:54PM L23.00006 2D patterned GaN$_{x}$As$_{1-x}$ Quantum structures using Ion Implantation and Pulsed Laser Melting, TAESEOK KIM, MICHAEL J. AZIZ, VENKATESH NARAYANAMURTI, School of Engineering and Applied Sciences, Harvard University — We will present two dimensionally patterned GaN$_{x}$As$_{1-x}$ nanostructures fabricated in a GaAs matrix using nitrogen implantation followed by pulsed laser melting and rapid thermal annealing (RTA). The arbitrarily patterned GaN$_{x}$As$_{1-x}$ regions are investigated by ballistic electron emission microscopy (BEEM), a three terminal scanning tunneling microscopy technique. BEEM can image both the surface topography and the local hot electron transport. By analyzing BEEM images, we are able to study the surface features for metal blackening and characterized the spectral responses of the black metals from UV to IR. The black metals promise potential for a variety of technologically important applications.

4:06PM L23.00007 Femtosecond laser-induced black metals, ANATOLIY VOROBYEV, CHUNLEI GUO, University of Rochester — Metals are one of the most commonly used materials in everyday life. One of the intrinsic properties of nearly all metals is that they are highly reflective for electromagnetic waves. Recently, by treating metal surfaces with high-intensity femtosecond laser pulses, we turned highly reflective metals highly absorptive and created, for the first time, “black metals”. We also investigated the surface features for metal blackening and characterized the spectral responses of the black metals from UV to IR. The black metals promise potential for a variety of technologically important applications.

4:18PM L23.00008 Cooling rates and mechanisms of resolidification in short pulse laser processing of metal targets1, LEONID ZHIGILEI, ZHIBIN LIN, WILLIAM DUFF, University of Virginia, DMITRIY IVANOV, Technical University of Kaiserslautern — Short-pulse laser irradiation of a metal target can create conditions for generation of non-equilibrium phases and unusual microstructure in the surface region of the irradiated target. The shallow melt depths produced by the short pulse laser irradiation and the high thermal conductivity of metals can result in very high cooling rates, strong undercooling and rapid resolidification. In this work, the melting and resolidification processes occurring under conditions of extreme heating and cooling rates are investigated in large-scale molecular dynamics simulations. The kinetics of the resolidification process and the microstructure of the surface region are found to be defined by a competition between the epitaxial regrowth of the substrate and nucleation of crystallites within the undercooled melt region. The dependence of the final microstructure of the surface region on the irradiation conditions is discussed.

1Financial support of this work is provided by the National Science Foundation, Grant No. CTS-0348503.

4:30PM L23.00009 Modeling of early-stage plasma during femtosecond laser ablation of metals, ZHAOYANG CHEN, SAMUEL MAO, UC Berkeley — We developed a model of early-stage plasma induced by intense femtosecond laser ablation of metals in an ambient gas. We consider a 100 fs FWHM, 800 nm wavelength laser pulse irradiating a copper target in 1 atm nitrogen environment. Electron and lattice temperature of laser-irradiated target were calculated based on a two-temperature model, with surface electron emission due to thermonic and photoelectric effects utilized as the boundary condition for plasma initiation. Plasma development was calculated based on conservation laws for electrons, ions, as well as atoms from ambient gas. Inverse Bremsstrahlung laser absorption by electrons and electron impact ionization were found to be responsible for plasma development, and the simulation results yielded the laser intensity threshold for femtosecond laser-induced plasma formation.
4:42PM L23.00010 Laser-Ablation Deposited Hafnium-Oxide Films for Triple Point Cathodes, RONALD GILGENBACH, NICHOLAS JORDAN, Y.Y. LAU, DAVID FRENCH, P. PENCVANICH, BRAD HOFF, MICHAEL ATZMON, University of Michigan — The triple-point is defined as the interface between metal, dielectric and vacuum; it provides a copious source of electrons for cold-cathodes. Pulsed-laser-deposition has been utilized to fabricate triple-point cathodes consisting of hafnium-oxide film-islands deposited over metal substrates. A 600 mJ, 20 ns KrF laser ablates a solid target of hafnium metal in a background gas of 20 percent O2 and 80 percent Ar at 100 mTorr at 10-15 ps. Contact lithography is employed to fabricate arrays of Hf-oxide islands on substrates to maximize the area of triple points for electron emission. For materials analysis, the films are deposited on a Si substrate. Plume plasma diagnostics include gated optical emission spectroscopy; neutral and singly-ionized hafnium have been measured. Hafnium-oxide film diagnostics include XEDS, SEM, TEM, profilometry, ellipsometry and x-ray diffraction (XRD). Hafnium-oxide deposition rates are about 0.06 nm/pulse. Cathode experimental current results will be presented at -300 kV.

1Research supported by AFOSR MURI on Cathodes & Windows for HPM and Applied Materials Corp.

4:54PM L23.00011 Growth control of GaAs nanowires using pulsed laser deposition with arsenic over-pressure, X.W. ZHAO, A.J. HAUSER, T. R. LEMBERGER, F.Y. YANG, Department of Physics, the Ohio State University — Using pulsed laser ablation with arsenic over-pressure, the growth conditions for GaAs nanowires (NWs) catalyzed by gold nanoparticles have been systematically investigated. The single-crystal structure and geometry of the NWs have been characterized for various growth conditions. Arsenic over-pressure with As2 molecules was introduced into the system by thermal decomposition of polycrystalline GaAs to control the stoichometry and shape of the NWs during growth. GaAs NWs exhibit a variety of geometries under varying arsenic over-pressures. Without As2 over-pressure, branched growth of GaAs with uncontrollable size and geometry was observed due to the decomposition of GaAs NWs, producing metallic Ga which serves as catalysts for the branched growth of GaAs on the nanowire surfaces. Under optimal As2 over-pressure, at substrate temperature of 570 °C, single-crystal GaAs NWs with uniform diameter of ~50 nm, small diameter distribution, length over 20 micrometers, and thin surface oxide layer of ~0.5 nm were obtained. X-ray diffraction results confirm the zinc-blende crystal structure of the GaAs NWs. A preliminary electrical characterization gives a linear J-V curve with a reasonable resistance, which leads to more thorough electrical characterization on GaAs NWs and device fabrication.


Tuesday, March 11, 2008 2:30PM - 5:30PM – Session L24 DMP: Focus Session: Transport in Nanostructures IV: 2DES, Dots, and QPCs

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2:30PM L24.00001 Coulomb and Spin Blockade transport through molecules and quantum dots, BHASKARAN MURALIDHARAN, Purdue University, OWEN MILLER, University of Virginia, AVIK GHOSH, Univeristy of Virginia, SUPRIYO DATTA, Purdue University — In this talk we address some common theoretical grounds between molecular electronics and quantum-dot transport. Here, we focus on how theoretical models based on Coulomb Blockade (CB) theory can be successfully applied in order to theoretically interpret various notable transport experiments in both molecular electronics and quantum dot transport. We first show that, a majority of low-temperature molecular experiments can be explained easily, using a simplified CB theory. In the later part, we focus on how the many-body excitation spectrum of the molecule/quantum dot plays a significant role, in many other experiments. This includes, not-so-commonly observed transport effects such as Negative Differential Resistance (NDR) and bi-stability, resulting from asymmetry within the molecule or within the quantum dot array.

2:42PM L24.00002 Influence of coherent level mixing on the resonant currents at anti-crossings between two single particle levels of a vertical quantum dot, C. PAYETTE, D.G. AUSTING, NRC, McGill University (Canada), G. YU, J.A. GUPTA, NRC (Canada), S.V. NAIR, University of Toronto (Canada), B. PARTOENS, Universiteit Antwerpen (Belgium), S. AMADA, ICORP-JST (Japan), Y. TAKURA, NTT-BRL (Japan), S. TARUCHA, ICORP-JST, University of Tokyo (Japan) — We study single electron resonant tunneling through weakly coupled vertical quantum dot molecules. Using the ground state of one of the constituent dots as an energy filter, we can probe the single particle energy spectrum of the other dot. Overall, the spectra are well modeled by assuming the dots are either circular or elliptical and parabolic, except in the regions where two or more single particle states approach each other. In these regions, we observe pronounced level mixing behavior. Here, we focus on the numerous two level anti-crossings, examining the conditions which lead to either simple transfer of the resonant current strengths between the two branches or concurrent enhancement and suppression of the resonant current in the two branches. We show that both types of behavior can be understood using a simple coherent level mixing model.

2:54PM L24.00003 Electron-Phonon Kinetics and Transport in 2D Structures of Reduced Electron Concentrations, ANDREI SERGEEV, SUNY at Buffalo, MICHAEL REIZER, VLADIMIR MITIN, SUNY at Buffalo — Usually, screening of the electron-phonon (e-ph) interaction is considered in linear approximation. In this case in 2D systems, the Debye screening radius \( r_D \) is independent on the electron concentration, \( n \). The linear approximation ignores the discreteness of the electron charge and it is not applicable for diluted systems. Here we show that the screening radius for e-ph interaction is in fact

\[
\max(r_D, n^{-1/2})
\]

For this reason, e-ph interaction is drastically enhanced in the diluted systems. In particular, a value of the deformation potential is increased by a factor of

\[
\frac{n^{1/2}}{r_D} \approx R_0/a_0 = r_s.
\]

The suggested approach explains puzzling data [1], which demonstrate that the deformation potential between holes and phonons in dilute 2D GaAs is twenty times stronger than expected from the theory. Strong coupling increases all e-ph phenomena. Using the Keldysh diagrammatic technique, we calculate kinetic and transport characteristics for diluted 2D systems. [1] X.P.A. Gao et al, Phys. Rev Lett. 94, 086402 (2005).

1The work was supported by the NYSTAR grant.
3:06PM L24.00004 Novel measurement techniques for probing quantum point contacts1 — LINDSAY MOORE, Stanford University — Conductance measurements of quantum point contacts (QPCs) reveal an anomalous plateau at roughly 0.7 x 2e^2/h, when the mode occupation is just short of making a fully transmitting 1D channel available. Past experiments have built a consensus that this so-called “0.7 structure” is related to electron spin and electron-electron interaction, but the detailed description remains controversial. We have performed measurements on two new kinds of devices which give new insight into the interactions of electrons in these clean quasi-one dimensional systems. One device allows us to measure the compressibility of the electrons in a QPC for the first several conduction modes. Comparison with density functional calculations give new information about the relative importance of interactions (including exchange) as the density in the QPC is depleted. The second device allows us to measure the local density of states (DOS) in the QPC as we tunnel directly into the constriction. Deviations from the 1D DOS would help to develop a more complete picture of the transport through a QPC. We acknowledge support from the ONR Young Investigator Program, Award No. N00014-01-1-0569 and a Research Corporation Research Innovation Award, No. R1260.

3:42PM L24.00005 Ballistic hole transport and the 0.7 anomaly in p-type GaAs quantum wires — A.R. HAMILTON, School of Physics, University of New South Wales, Sydney, NSW 2052, Australia, R. DANNEAU, UNSW and Low Temperature Laboratory, Helsinki University of Technology, Espoo, Finland, O. KLOCHAN, W.R. CLARKE, L.H. HO, A.P. MICOLICH, M.Y. SIMMONS, School of Physics, University of New South Wales, Sydney, NSW 2052, Australia, M. PEPPER, D.A. RITCHIE, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, U.K. — Studying the spin degree of freedom of charge carriers in semiconductors is an area of significant current interest. Although spin-orbit coupling is extremely strong in p-type semiconductors such as GaAs, to date there have been only a limited number of experiments on holes in p-GaAs nanostructures. We have fabricated extremely high quality 1D hole quantum wires that show up to 10 extremely clean and stable quantized conductance plateaus at B=0 [1]. In contrast to 1D electrons, we observe an extreme anisotropy of the Zeeman spin splitting of the 1D energy levels depending on whether the magnetic field is parallel or perpendicular to the quantum wire [2]. We use this anisotropy to show that the 0.7 feature and zero bias anomaly are both spin related in hole quantum wires [3]. [1] O. Klocham et al, APL 89, 092105 (2006); R. Danneau et al, ibid 88, 012107 (2006). [2] R. Danneauet al, PRL 97, 026403 (2006). [3] R. Danneau et al, PRL in press.

3:54PM L24.00006 Elementary Events of Electron Transfer in a Voltage-Driven Quantum Point Contact — MIHAJLO VANEVIC, YULI NAZAROV, WOLFGANG BELZIG, Universitat Basel — We find that the statistics of electron transfer in a coherent quantum point contact driven by an arbitrary time-dependent voltage is composed of elementary events of two kinds: unidirectional one-electron transfers determining the average current and bidirectional two-electron processes contributing to the noise only. This result pertains at vanishing temperature while the extended Keldysh-Green’s function formalism in use also enables the systematic calculation of the higher-order current correlators at finite temperatures.

4:06PM L24.00007 Zeeman splitting and subband spacing in ballistic Ga0.25In0.75As/InP quantum point contacts — THEODORE MARTIN, A. SZORKOVSKZY, University of New South Wales, C.A. MARLOW, University of Oregon, L. SAMUELSON, Lund University, H. LINKE, University of Oregon, R.P. TAYLOR, University of Canterbury, A.P. MICOLICH, A.R. HAMILTON, University of New South Wales — Spin-resolved transport in low-dimensional, solid state systems is a leading area of research at the nanoscale, due to potential device applications. This project extends our work in the quantization of such devices using the spin-orbit coupling to generate a well-resolved energy level spectrum and a large splitting of the spin-degeneracy. Here we investigate the transport properties of a ballistic quantum point contact (QPC) etched into a high indium content strained GaInAs/InP heterostructure, a system with strong spin-orbit coupling and large 1D subband spacings. We have measured the 1D subband spacing using two independent methods, and find it to be ~10 meV, with a very steep confining potential. We also present data studying the Zeeman splitting of the 1D subbands for different magnetic field orientations.

4:18PM L24.00008 Magnetococonductance of interacting electrons in quantum wires in the integer quantum Hall regime — IGOR ZOZOLENKOV, SIARHEI HNATSENKA, Linkoping University — We present systematic quantitative description of the magnetococonductance of the split-gate quantum wires. Accounting for the exchange and correlation interactions within the spin density function theory (DFT) leads to the lifting of the spin degeneracy and formation of the spin-resolved plateaus at odd values of e^2/h. We show that the width of the odd conductance steps in the spin DFT calculations is equal to the width of the transition intervals between the conductance steps for the spinless Hartree electrons. A detailed analysis of the structure of compressible/incompressible strips and the evolution of the Hartree and the spin-DFT subband structure provides an explanation of this finding. Our spin-DFT calculations reproduce not only qualitatively, but rather quantitatively all the features in the magnetoconductance observed in the experiment [1] including the unexpected effect of the collapse of the odd conductance plateaux at lower fields.

4:30PM L24.00009 The Virtual Scanning Tunneling Microscope: A Novel Probe Technique for Imaging Two-Dimensional Electron Systems — ADAM SCIAMBI, DAVID GOLDBERGER-GORDON, Stanford University, SETH BANK1, ARTHUR GOSSMARK, University of California, Santa Barbara — We propose a novel probe technique, the virtual scanning tunneling microscope (VSTM), which will provide both spatial and spectroscopic information about two-dimensional electron systems (2DESs) in semiconductor heterostructures. The VSTM’s innovation is the addition of a second ‘probe’ 2DES separated by a low barrier from the sample 2DES below. Simulations show that a positively-biased tip held above the sample surface can greatly diminish the interlayer barrier and induce tunable tunneling between the two 2DESes. If the tip is scanned, the tunneling region will follow below, acting as a virtual tip while screening the true tip from the sample 2DES. This probe technique is motivated by interesting local 2DES physics that can only be studied indirectly because of the depth of 2DESes; we describe a range of predicted spatially-organized phases of 2D electrons which could be accessed with this new probe. We follow with experimental results showing induced tunneling in a GaAs/AlGaAs bilayer 2DES sample, which we characterize thoroughly and use to tunnel into a quantum Hall liquid.

4:42PM L24.00010 Virtual Scanning Tunneling Microscope: Modeling Interlayer Tunneling Between Two-Dimensional Electron Systems in the Ballistic Regime — KATHERINE LUNA, EUN-AH KIM, PAUL ORETO, STEVEN KIVELSON, Stanford University — We study a theoretical model for the virtual scanning tunneling microscope (VSTM), which is a proposal to use interlayer tunneling in a bilayer system as a way to probe two-dimensional electron systems (2DES) in semiconductor heterostructures. We moderate the bi-layer in the presence of weak tunneling between the layers using an analog of the spin-boson model. Previously, such a system was modeled in the diffusive regime by Levitov and Shytov [1], and they predicted a zero-bias anomaly, where the tunneling conductance vanishes singularly near zero-bias as a result of Coulomb blocking. Motivated by the availability of high mobility samples and the goal of using VSTM to probe the physics of clean 2DES dominated by interactions, we focus on tunneling in the ballistic regime. We find the absence of a zero-bias anomaly due to extremely efficient screening in the ballistic regime. We discuss the implications of our results on ongoing experimental efforts. [1] S. Levitov and A.V. Shytov. JETP Lett. 66, 214 (1997).
enhance the formation of lamellar structure consisting of the alpha-form of isotactic polypropylene (iPP) crystal. At low temperature (e.g., polymer in melts, the confinement to the layers results in an enhanced gamma form where hydrogen bonds form in between parallel nylon 6 chains dominate. Interface with the clay particles, the polymer chains orient perpendicular to the interface. While the alpha crystalline form dominated the structure of the polymer in the nano-particle. The structural evolution as a result in alternating layers of nylon and nylon/clay regions forming two distinct interfaces, that with the nanocomposites made by chaotic flow. 

Optical, and electrical applications. Single crystal lattice, tethering them to both surfaces. This control over the 2D assembly of these materials allows us to study materials for various biological, optical, and electrical applications.

5:06PM L25.00002 Polymer Single Crystals as 2D Templates. STEPHEN CHENG, RYAN VAN HORN, WENBIN ZHANG, University of Akron — Polymer single crystals grown from dilute solution provide a novel approach to studying polymer physics. Because these crystals are lamellar in shape, their fold surfaces provide a platform from which to study two-dimensionally ordered structures. By coupling other polymers (forming multiblock copolymers) or inorganic particles (forming organic/inorganic hybrids) to the crystallizable block, it is possible to analyze the inherent physics of confining this assembly to 2D space and to provide an opportunity to use the crystal as a template. These non-crystallizable components are excluded from the single crystal lattice, tethering them to both surfaces. This control over the 2D assembly of these materials allows us to study materials for various biological, optical, and electrical applications.

5:18PM L25.00013 ABSTRACT WITHDRAWN –
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5:06PM L25.00001 Dillon Symposium Break –

3:06PM L25.00002 Polymer Single Crystals as 2D Templates. STEPHEN CHENG, RYAN VAN HORN, WENBIN ZHANG, University of Akron — Polymer single crystals grown from dilute solution provide a novel approach to studying polymer physics. Because these crystals are lamellar in shape, their fold surfaces provide a platform from which to study two-dimensionally ordered structures. By coupling other polymers (forming multiblock copolymers) or inorganic particles (forming organic/inorganic hybrids) to the crystallizable block, it is possible to analyze the inherent physics of confining this assembly to 2D space and to provide an opportunity to use the crystal as a template. These non-crystallizable components are excluded from the single crystal lattice, tethering them to both surfaces. This control over the 2D assembly of these materials allows us to study materials for various biological, optical, and electrical applications.

3:18PM L25.00003 Interfacial and confinement effects to the structure of nylon 6 /clay nanocomposites made by chaotic flow. DILRU RATNAWEERA, DVORA PERAHIA, CHAITRA MAHESHA, DAVID ZUMBRUNNEN, Clemson University, MARK KAMPF, Appelton — The structure of polymers within nanocomposites is strongly affected by the confinement of the polymer to the interface with the nanoparticles and the method of blending. In nanocomposites of Nylon 6 and clay particles are made by chaotic blending, the strength of the chaotic flow affects the internal structure on multiple length scales, where the local structure is determined by the interfacial effects between the polymer and the nano-particle. The structural evolution as a results in alternating layers of nylon and nylon/clay regions forming two distinct interfaces, that with the clay and that of the pure nylon and the composite. The structure has been studied by X-ray, AFM and TEM at different chaotic blending strengths. At the interface with the clay particles, the polymer chains orient perpendicular to the interface. While the alpha crystalline form dominated the structure of the polymer in melts, the confinement to the layers results in an enhanced gamma form where hydrogen bonds form in between parallel nylon 6 chains dominate.

3:30PM L25.00004 WAXS investigations on Polyethylene – Carbon Nanofibers Composites. BRIAN JONES, University of Nebraska, Lincoln, JIANHUA LI, Rigaku Americas, TX, ROGELIO BENITEZ, KAREN LOZANO, MORCEA CHIPARA, ALIN CRISTIAN CHIPARA, MAGDALENA DOGNA CHIPARA, The University of Texas Pan American, DAVID J. SELLMYER, University of Nebraska, Lincoln — Nanocomposites have been obtained by high-shear mixing of isotactic polyethylene with various amounts of purified nanofiller (vapor grown carbon nanofibers type PR-24AG from Pyrograf Products, Inc) by utilizing a HAAKE Rheomix at 65 rpm and 180 °C for 9 min followed by an additional mixing at 90 rpm for 5 min. Composites loaded with various amount of vapor grown carbon nanofibers have been prepared. Various spectroscopic techniques have been used to assess the interactions between the polymeric matrix and carbon nanofibers. Wide angle X - Ray scattering investigations focused on the effect of carbon nanofibers on the crystalline phases of polypropylene and on the overall crystallinity degree of the polymeric matrix. This research aims at a better understanding of the nature and structure of the polymer – carbon nanofibers interface.

3:42PM L25.00005 Crystallization of Propylene-Hexene Random Copolymer. YIMIN MAO, FENG ZUO, JONGKAHK KEUM, BENJAMIN HSIAO, Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400 — Time resolved small- and wide-angle x-ray scattering (SAXS/WAXS) were used to study the crystallization behavior of propylene-hexene random copolymer containing non-crystallizable hexene segments and crystallizable propylene segments. It was found that the copolymer would follow two crystallization paths depending on temperature, resulting in two distinct crystalline structures. At high crystallization temperatures (e.g. 100°C), the combined effects of phase separation and high chain mobility greatly enhance the formation of lamellar structure consisting of the alpha-form of isotactic polypropylene (iPP) crystal. At low temperature (e.g. 40°C), the lack of phase separation and the low chain mobility mainly result in the formation of fringe-micelle structure also with the alpha-form of iPP.

3:54PM L25.00006 Probing the crystallisation of polyethylene confined to a system of droplets. JESSICA CARVALHO, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — We present results on the crystallisation of polyethylene (PE) confined to a system of dewetted droplets. With the droplet system, we have access to a large ensemble of small. isolated volumes of crystallisable material, allowing for a direct measurement of nucleation rates. In our previous work with dewetted droplets of poly(ethylene oxide), we were able to demonstrate that long chains showed the same nucleation behaviour as chains roughly an order of magnitude shorter[1]. In contrast to this, it has been shown that for systems of n-alkanes molecular weight plays a role[2]. By investigating a wide range in molecular weight, the dependence of nucleation on molecular weight will be addressed in PE. [1] M.V. Massa et al., Phys. Rev. Lett. 97, 247802 (2006). [2] H. Kraack et al., Macromolecules, 33, 6174 (2000).
4:06PM L25.00007 Crystalline Morphology of Propylene 1-Octene Random Copolymers¹. KEEsu JEOu, RUFUINA G. ALAmO, Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering — The morphology of isotactic propylene 1-octene random copolymers has been studied by AFM, DSC, WAXS, and FTIR in an octene range of 10-20 mol %. Different morphologies were observed below and above 15 mol %. The morphological components in the higher count copolymers are not of the lamellae-type, thicker than lamellae observed below 15 mol %, connected and isotropic in their orientation. Their global morphology is developed via nucleation and growth (NG) of spherulitic aggregates. The evolution of heat of fusion with time is also sigmoidal shape, typical of NG-type crystalization mechanism. WAXS diffractograms for the higher count copolymers are devoid of crystalline reflections, except for small and broad peaks suggesting mesomorphic-like structures, which by FTIR show small contents of the 840 cm⁻¹, 12 and higher units regularity bands, and hence formed of short helical sequences. The PO morphology is additionally compared with copolymers with ethylene, 1-butene and 1-hexene counts at matched contents.

¹Work supported by NSF-DMR-0503876.

4:18PM L25.00008 Tailoring the Properties of Poly(ethylene terephthalate) without Addition of Fillers via Solid-State Shear Pulverization. CYNTHIA PIERRE, KOSMAS KASIMATIS, JOHN TORKELSON, Northwestern University — We demonstrate the ability to very strongly tune the physical and mechanical properties of poly(ethylene terephthalate) (PET) by changing the processing conditions of neat PET during solid-state shear pulverization without addition of any fillers or nucleating agents. Using differential scanning calorimetry, we observe a roughly factor of 3 increase in crystallinity of PET that has been pulverized and subsequently melted relative to the unprocessed PET. We also observe a dramatic increase in the rate of crystallization of the pulverized samples. Rheological characterization has demonstrated an increase in viscosity of the pulverized material, which can be ascribed to branching in the pulverized product. We also observe significant reductions in the oxygen permeability of the PET with pulverization as well as enhancements in mechanical properties that are commensurate with the modified crystallization properties of the pulverized PET.

4:30PM L25.00009 Crystallization of Bromine Substituted Polyethylene with Precise Placement or Random Distribution¹. R.G. ALAMO, K. JEOU, R.L. SMITH, FAMU-FSU College of Engineering, E. BOZ, K.B. WAGENER, Dept. of Chemistry, University of Florida — The crystalline properties of a series of bromine containing polyethylene (PEs) with either a random or an exact placement of the Br atom on each and every 21st, 19th, 15th and 9th backbone carbon have been studied by DSC, NMR, Raman spectroscopy, WAXS and SAXS. Taking into account a larger strain due to the size of the Br atom, the crystallization behavior is analogous to Cl substituted PEs. While all precision Br-PEs crystallize as homopolymers as demonstrated by 1. DMDAS solid-state ¹³C NMR spectra; 2. development of relatively large crystal thickness, and 3. sharp crystallization and melting peaks, the development of the crystalline state in random analogues is led by selection of most crystalline sequences indicated by broad thermal transitions, and lower crystallinities. WAXS patterns are unique for each type of substitution. For precision Br-PEs WAXS contain reflections corresponding to planes containing the Br atoms which are tilted 35° in reference to the chain axis. Due to the accommodation of the large Br atom, the crystals of all precisely substituted Br-PEs studied are deformationally disordered as observed by their Raman and NMR spectra. In contrast, crystals from random analogues display negligible conformational disorder.

¹Work supported by NSF-DMR-0503876.

4:42PM L25.00010 Molecular and Crystalline Microstructure of Ferroelectric Poly(vinylidene fluoride-co-trifluoroethylene) Ultrathin Films on Bare and Self-Assembled Monolayer-Modified Au Substrates. YOUN JUNG PARK, SEOK JU KANG, Yonsei University, BERNARD LOTZ, ANNETTE THIERRY, Institut Charles Sadron, CHEOLMIN PARK, Yonsei University — There has been much interest in polymorphic crystal structures and ferroelectric properties in polymer materials, as one way of an application for organic memory device. We investigate the molecular and microdomain structure of Poly vinylidene fluoride-co-trifluoroethylene (P(VDF-TrFE)) thin films spin-coated on bare and self-assembled monolayers (SAMs)-modified Au substrates. The two types of films display similar crystalline morphologies with edge-on needlelike crystalline microdomains. They have, however, a different structure depending on the substrate. When the films are deposited on a bare Au surface, the films preferentially have a (110) contact plane with the substrate but a (100) contact plane when deposited on the Au surface modified by SAMs. The polar b-axis, along which the ferroelectric polarization is oriented, is therefore tilted to the film (and substrate) surface normal at 30 and 90°, respectively. In particular, the orientation of the polar b-axis tilted at some 90° to the normal of the polymer films on a CH₃ terminated SAM modified Au surface explains the smaller remanent polarization at low initial electrical bias.

4:54PM L25.00011 Chirality Information Transfer in Poly(Lactides): From Main-Chain Chirality to Lamella Curvature. ROBERT EMERY PRUD’HOMME, DAMIEN MAILLARD, University of Montreal — The behaviour of ultrathin polymer films is very different from that in the bulk phase. In this work, the crystallization of poly(D-lactide) (PDLa) and poly(L-lactide) (PLLa) was followed using in situ atomic force microscopy over a broad range of temperatures and thicknesses. Using a forced nucleation technique, edge-on lamellae were observed, showing a curvature which can be related to the polymer chirality. In the case of PLLA, the lamellae are S-shaped, contrary to the PDLa lamellae which are Z-shaped. This behaviour was also observed on TEM pictures of PLLA and PDLA films crystallized in the same conditions without any external nucleation. For the first time, a relationship has been established between the molecular chirality of poly(lactide)s and their macroscopic behaviour. Moreover, the rotating direction of those lamellae can be directly linked with the sense of twisting of the poly(lactide)s lamellae in banded spherulites. Those observations can lead to a model to where the curved crystals in ultrathin films can be considered as half-lamellae, which, when associated together, give twisted complete lamellae.

5:06PM L25.00012 Effects of Vitamin E on the Oxidative Reaction of Free Radicals in Ultra-High Molecular Weight Polyethylene. BENJAMIN WALTERS, MUHAMMAD JAHAN, The Univ. of Memphis, Phys Dept. — Free radicals in gamma- or x-irradiated ultra-high molecular weight polyethylene (UHMWPE) are investigated as a function of vitamin E (alpha-tocopherol (α-T)). α-T is mixed with UHMWPE (GUR 1020) powder (e-PE) before (premix) or after (post-mix) irradiation. Pre-mix powder is also compression-molded (CM) to solid pucks (1" thick and 2.5" dia.) at 200°C under constant force of 20-40 kN. Free radicals are detected using an X-band electron spin resonance (ESR) spectrometer, and oxidation index (OI) (1720 cm⁻¹) by FTIR technique. As expected, no measurable OI is detected by FTIR and thus e-PE suffers no loss in its mechanical properties. ESR data, however, suggest that α-T quenches polyethylene radicals during and/or immediately after irradiation, but it does not have any effect on the long-term oxidative reaction. The difference between the pre- and post-mix powder is apparent only at the initial stage, and the terminal oxygen-induced radicals (OIR) are produced in all irradiated samples. Both pre- and post-mix powders are found to have equal amount of residual α-T radical (tocophereryl).
is difficult. Limit the number of control electrodes due to the constraints of size, decoherence and cross-talk, and where complex temporal variation of the control voltages of the ‘quantum wire’ and the system’s symmetries are explored. It may also be relevant for gate-controlled solid-state systems where it is desirable or necessary to show how such minimal control could significantly improve information processing in terms of speed, fidelity and transfer efficiency. The scheme presented has efficient execution of a range of useful QIP tasks. We show that it is in principle possible to achieve global control with a single, simple, fixed, local actuator, and most restricted candidate systems where only a single energy transition can be controlled by a piecewise-constant field, and show that even this is sufficient for viable control solution. Normal optimization problems in virtually any area of engineering and science typically have landscape topologies that remain a mystery. Quantum mechanics appears out to be quite special in that the topology of quantum control landscapes can be established generically based on minimal physical assumptions. Various features of these landscapes will be discussed and illustrated for circumstances where the controls are either an external field or the time independent portions of the Hamiltonian; the latter circumstance corresponds to subjecting the material or molecules to systematic variation and hence viewed in the context of being controls. Both theoretical and experimental findings on control landscapes and their consequences will be discussed, including issues of robustness to noise, search algorithm efficiency, existence of multiple control solutions, prospects for identifying reduced sets of control variables, simultaneous control of multiple quantum systems (optimal dynamic discrimination (ODD)), and mechanism analysis.

 Seeking the best control over a posed quantum dynamic objective entails climbing over the associated control landscape, which is defined as the quantum mechanical observable as a function of the controls. The topology and general structure of quantum control landscapes as input output maps dictate the final attainable yield, the efficiency of the search for an effective control, the possible existence of multiple dynamically equivalent controls, and the robustness of any viable control solution. Normal optimization problems in virtually any area of engineering and science typically have landscape topologies that remain a mystery. Quantum mechanics appears out to be quite special in that the topology of quantum control landscapes can be established generically based on minimal physical assumptions. Various features of these landscapes will be discussed and illustrated for circumstances where the controls are either an external field or the time independent portions of the Hamiltonian; the latter circumstance corresponds to subjecting the material or molecules to systematic variation and hence viewed in the context of being controls. Both theoretical and experimental findings on control landscapes and their consequences will be discussed, including issues of robustness to noise, search algorithm efficiency, existence of multiple control solutions, prospects for identifying reduced sets of control variables, simultaneous control of multiple quantum systems (optimal dynamic discrimination (ODD)), and mechanism analysis.

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This work was supported by NSF CAREER Award DMR-0348724.

Tuesday, March 11, 2008 2:30PM - 5:18PM - Session L26 DCP: Focus Session: Quantum Control II

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2:30PM L26.00001 Hiking Over Quantum Control Landscapes, HERSCHEL RABITZ, Princeton University — Seeking the best control over a posed quantum dynamic objective entails climbing over the associated control landscape, which is defined as the quantum mechanical observable as a function of the controls. The topology and general structure of quantum control landscapes as input output maps dictate the final attainable yield, the efficiency of the search for an effective control, the possible existence of multiple dynamically equivalent controls, and the robustness of any viable control solution. Normal optimization problems in virtually any area of engineering and science typically have landscape topologies that remain a mystery. Quantum mechanics appears out to be quite special in that the topology of quantum control landscapes can be established generically based on minimal physical assumptions. Various features of these landscapes will be discussed and illustrated for circumstances where the controls are either an external field or the time independent portions of the Hamiltonian; the latter circumstance corresponds to subjecting the material or molecules to systematic variation and hence viewed in the context of being controls. Both theoretical and experimental findings on control landscapes and their consequences will be discussed, including issues of robustness to noise, search algorithm efficiency, existence of multiple control solutions, prospects for identifying reduced sets of control variables, simultaneous control of multiple quantum systems (optimal dynamic discrimination (ODD)), and mechanism analysis.

3:06PM L26.00002 Non-resonant, non-perturbative Dynamic Stark Control of Quantum Dynamics, ALBERT STOLOW, National Research Council — One of the most important non-resonant interactions is the dynamic Stark effect. In the non-resonant but non-hamiltonizing limit, an effective Hamiltonian can be constructed based upon a hierarchy of approximations (the Born-Oppenheimer Approximation, Slowly Varying Envelope Approximation, the Rotating Wave Approximation). In this situation, the effective Hamiltonian contains first order (dipole) and second order (polarizability) matter-field interactions which can lead to significant yet reversible changes to the molecular Hamiltonian. The first order term leads to a fast evolution which follows each optical cycle. The second order term causes an evolution which follows, by contrast, the envelope of the laser pulse. We discuss the use of the non-resonant second order Dynamic Stark Effect as a tool for controlling quantum systems without any net absorption of light. We illustrate this by examples chosen from problems in: (i) Control of branching ratios during non-adiabatic photodissociation; (ii) Control of 3D field free molecular frame alignment of asymmetric tops.

3:42PM L26.00003 Controlling and Understanding Laser Filamentation in the Solution and Gas Phase Molecular Systems, ROBERT J. LEVIS, Temple University — The process of laser filamentation is highly nonlinear, yet amenable to control using laser pulse shaping techniques. Investigations of our ability to control the spatial position of a filament in a water tank and measurements of the forward and back scattered amplified spontaneous emission (resulting from the strong field excitation in the resulting plasma) will be presented. Our time resolved measurements of the dynamics of the filamentation process in various gases will also be reviewed. Finally, a model of the plasma formation will be presented.

4:18PM L26.00004 New Developments in Quantum Control: Phase Space Learning Algorithms and Uncontrollable Quantum Systems, DAVID J. TANNOR, Department of Chemical Physics, Weizmann Institute of Science — This talk has two parts. The first deals with a new representation of shaped ultrafast laser pulses based on a von Neumann time-frequency lattice. We show that a pulse defined in terms of an amplitude and a phase at N frequency points can be represented on the von Neumann lattice using √N points in frequency and √N in time without loss of information. The transformation from the frequency (or time) representation to the von Neumann representation is one-to-one and therefore invertible. We discuss three possible applications of the von Neumann representation of pulses: 1) for cleaning and interpreting complex pulses; 2) for performing systematic scans of the effect of timing and frequency on molecular control; 3) as genes to be used in mutations and crossover in evolutionary algorithms. The second part of the talk deals with the classification of uncontrollable quantum systems. It is well-known that for a quantum system to be controllable the Lie algebra spanned by iterated commutators of H0 and H1 must span the full space of the dynamical algebra. We pose the following questions: When a system is not completely controllable, can we classify different families of uncontrollable systems? If so, can we associate these different types of mathematical structures with different underlying physics (for example, dark states or generalized entangled states)? We show that uncontrollable quantum systems fall into two categories: reducible and irreducible. The former is associated with dark states and the latter with generalized entangled states. Based on Lie subalgebras we give a complete characterization of irreducible uncontrollable systems for systems up to 9 levels. Finally, we show that an earlier intuitive concept of connectivity only incompletely captures this Lie algebraic structure of uncontrollable systems.

1The first part of this work was done in collaboration with Susanne Fechner, Frank Dimler, Tobias Brixner, and Gustav Gerber, University of Wuerzburg. The second part was done in collaboration with Thomas Polack and Haim Suchowski, Weizmann Institute.

4:54PM L26.00005 Quantum information processing with a minimal control, PETER PEMBERTON-ROSS, SONIA SCHIRMER, DAMTP, University of Cambridge, IVAN PULLEN — Various physical and practical constraints limit the amount and type of control we have in quantum information processing systems, leading to complicated or unreliable implementations. To try and circumvent these problems, we take the most restricted candidate systems where only a single energy transition can be controlled by a piecewise-constant field, and show that even this is sufficient for efficient execution of a range of useful QIP tasks. We show that it is in principle possible to achieve global control with a single, simple, fixed, local actuator, and show how such minimal control could significantly improve information processing in terms of speed, fidelity and transfer efficiency. The scheme presented has a natural application to spin-chain systems, where only one interaction between two spins can be controlled, and the effects of the position of the controller in the ‘quantum wire’ and the system’s symmetries are explored. It may also be relevant for gate-controlled solid-state systems where it is desirable or necessary to limit the number of control electrodes due to the constraints of size, decoherence and cross-talk, and where complex temporal variation of the control voltages is difficult.
A Simulation of Strong-Field Attosecond Electron Dynamics: Effects of Pulse Shape

Tuesday, March 11, 2008 2:30PM - 5:30PM — Session L27 GMAG: Focus Session: Low-dimensional Spin Systems

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2:30PM L27.00001 Specific heat and magnetoelectric effect of the S=1/2 spin-ladder compound (CH$_3$)$_2$CHNH$_3$CuCl$_3$ , YOUNGHAK KIM, YASUO YOSHIDA, YASUMASA TAKANO, University of Florida, HIROYUKY TSUJII, Kanazawa University, KEISHI KANADA, TAKEHIRO SAITO, AKIRA OOSAWA, TAKAYUKI GOTO, Sophia University — As the complexity of systems increases from atoms to molecules, the exploration of non-adiabatic electron dynamics in strong fields requires a leap in understanding and in the principles of description. Recently, a time-dependent Hartree-Fock approach (TDHF) was developed to study the dynamics of individual electrons in multielectron systems. We have used this TDHF approach to numerically simulate the non-adiabatic electron dynamics of a few small molecules and polyacenes using basis sets ranging from AUG-cc-pVTZ for smaller molecules to 6-31G(d,p) for larger molecules. The electric field was applied in the direction of the long molecular axis and the attosecond response of the electrons during and after the laser pulse has been obtained. To determine the effects of ionization, electron dynamics for both neutrals and ions was also simulated. As a function of pulse shape, there are significant differences in the excitation spectrum and volume for each molecule.

2:42PM L27.00002 Neutron scattering study of strong- and weakly-coupled, spin-1/2 spin-ladders , BELLA LAKE, S. NOTBOHM, D.A. TENNANT, Hahn-Meitner Institut, T.G. PERRING, C.D. FROST, R.I. BEWLEY, P. MANUEL, K.P. SCHMIDT, G.S. UHRIG, P. RIBEIRO, C. SEKAR, R. KLINKELER, C. HESS, G. KRABBES — This presentation will discuss two-leg spin-ladders where the magnetic ions have spin-1/2 moments and antiferromagnetic exchange interactions. In the limit of strong rung coupling, the magnetic spectrum is dominated by the gapped magnon mode of an antiferromagnetic dimer, introduction of leg coupling modulates this mode. In the limit of weak rung coupling the excitations are similar to the multi-spinon continuum of the one-dimensional, spin-1/2, Heisenberg antiferromagnet, although the gap remains in the presence of infinitesimal rung coupling. Cyclic exchange interactions are often found in spin-ladders and reduce the gap size. Inelastic neutron scattering measurements will be presented for two ladders. La$_2$Sr$_{10}$Cu$_{24}$O$_{41}$ has strong rung coupling and excitations consisting of a gapped one-magnon mode and a two-magnon continuum. In contrast CaCu$_2$O$_3$ has a weak rung interaction and a substantial cyclic exchange which drives the system gapless and quantum critical. The excitations are similar to a multi-spinon continuum of a spin-1/2 chain, however the presence of rung coupling is revealed by a modulation parallel the rung at low energies.

3:06PM L27.00004 Magnetic and transport properties of the mixed valent vanadium oxides LuV$_4$O$_8$ and YV$_4$O$_8$ — S. DAS, A. NIAZI, D.C. JOHNSTON, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011 — Mixed valent vanadium oxides have been subjects of wide interest owing to their exotic properties such as heavy fermion behavior below 10 K in spinel LuV$_4$O$_8$, isomorphous phase transition and charge ordering in YbV$_4$O$_8$, LuV$_4$O$_8$ (L = Y, Lu) crystallize in a structure similar to that of orthorhombic CaFe$_2$O$_4$, containing four inequivalent V sites arranged in zig-zag chains. The formal oxidation state of V in these compounds is 3.25. In this study, the magnetic and transport properties of these LuV$_4$O$_8$ compounds are reported. The magnetic susceptibility indicates two possible structural phase transitions in YbV$_4$O$_8$ in the temperature (T) range 70–90 K. Anomalies in the heat capacity are also seen in this temperature range. The zero- field-cooled/field-cooled magnetic susceptibilities show possible canted antiferromagnetic ordering in both YbV$_4$O$_8$ and LuV$_4$O$_8$ for T < 50 K. For LuV$_4$O$_8$, the dc electrical resistivity of a sintered pellet measured using a standard four-probe technique shows a strong increase at T < 100 K. Supported by the USDOE under Contract No. DE-AC02-07CH11358.

3:18PM L27.00005 Single Crystal Growth and Characterization of Quasi 1-D, Magnon BEC Candidate Pb$_2$V$_3$O$_9$ , BENJAMIN CONNER, NHMFL/FSU, WANG ZHANG, NHMFL, CHRISTOPHER WIEBE, NHMFL/FSU, LUIS BALICAS, YOUNG-JUNG JO, NHMFL — Recent success in the floating zone growth of single crystal Pb$_2$V$_3$O$_9$ will be highlighted. Pb$_2$V$_3$O$_9$ has been studied as part of the class of antiferromagnetic 1D spin 1/2 dimer compounds that are believed to be driven through a phase transition to a BEC state with applied magnetic field. Magnetic susceptibility and specific heat measurements will be discussed.

3:30PM L27.00006 Magnetic structure of frustrated Haldane chain compound Ca$_2$V$_4$O$_7$ , B. LAKE, Hahn-Meitner Institut, O. PIPER, A. DAVOLD-LADINE, M. REEHUIS, K. PROKES, M. EINERLE, A. NIAZI, J.Q. YAN, D.C. JOHNSTON — While the Haldane chain, (Heisenberg spin-1 chain with nearest neighbor antiferromagnet interactions) has been much studied and shown to have gapped magnon excitations, the effect of frustration and single ion-anisotropy has not been investigated experimentally. Theory suggests that frustration can enhance the multi-particle spectrum and the combination of frustration and anisotropy can drive the system into a gapless chiral phase. Ca$_2$V$_4$O$_7$ is a candidate for such a system. This compound consists of two inequivalent one-dimensional chains consisting of spin-1 V$^{3+}$ ions which have antiferromagnetic first and second neighbour interactions. Interchain coupling gives rise to long-range order below $T_g$ = 71K. Neutron diffraction measurements will be described. They reveal collinear spin order within the chains and canting between chains, with the average spin direction along the $b$ axis. The ordered spin moment was also measured and found to be 1 $\mu_B$ per Vanadyl; this reduction of 50% from full spin ordering suggests loss of moment due to quantum fluctuations. Finally, preliminary inelastic neutron scattering reveals a gap due to single-ion anisotropy. In addition a steep dispersion along the $c$ (chain) direction and much weaker dispersions along $a$ and $b$ confirm the one-dimensional nature of Ca$_2$V$_4$O$_7$. Supported by the USDOE under Contract No. DE-AC02-07CH11358.
The local density of states of a finite quantum wire: New insights from DMRG and bosonization

We consider interacting fermions on a finite one-dimensional lattice. By using an adapted DMRG algorithm we are able to calculate the energy and spatially resolved local density of states (LDOS) for the lattice model directly without using time-dependent correlations. We compare to analytic expressions for individual energy levels in systems with open boundary conditions from Luttinger Liquid theory. In this way, a detailed understanding of the LDOS for each individual energy level can be obtained in both fermionic and bosonic pictures. Certain degeneracies of the Luttinger Liquid spectrum are lifted in the lattice model by band curvature and interaction effects, leading to a large number of states and energy levels in the LDOS. The standing waves in the LDOS reveal the collective bosonic excitations explicitly.

Real-time dynamics of spinons and holons in one-dimensional correlated electron systems

In the antiferromagnetic spin-liquid spin-wave stiffness and the Isinglike ferromagnetic excitation spectrum gap, exhibiting the spin-wave to spinon crossover. In the group theory, throughout the entire temperature and anisotropy ranges in both ferromagnetic and antiferromagnetic regions. We obtain, for all anisotropies, the in-plane interaction $s_{i}^z s_{j}^z + s_{i}^x s_{j}^x$ induces an antiferromagnetic correlation in the out-of-plane $s_{i}^y$ component. Conversely, an antiferromagnetic $s_{i}^z s_{j}^z$ interaction induces an correlation in the $s_{i}^x$ component. As another purely quantum effect, (i) in the antiferromagnet, the value of the specific heat peak is insensitive to anisotropy and the temperature of the specific heat peak decreases from the isotropic (Heisenberg) with introduction of either type (Ising or XY) anisotropy; (ii) in complete contrast, in the ferromagnet, the value and temperature of the specific heat peak increase with either type of anisotropy.

Excitation Spectrum Gap and Spin-Wave Stiffness of XXZ Heisenberg Chains: Global Renormalization-Group Calculation

The anisotropic XXZ spin-$\frac{1}{2}$ Heisenberg chain is studied using renormalization-group theory, throughout the entire anisotropy ranges in both ferromagnetic and antiferromagnetic regions. We obtain, for all anisotropies, the in-plane interaction $s_{i}^z s_{j}^z$ + $s_{i}^x s_{j}^x$ induces an antiferromagnetic correlation in the out-of-plane $s_{i}^y$ component. Conversely, an antiferromagnetic $s_{i}^z s_{j}^z$ interaction induces an correlation in the $s_{i}^x$ component. As another purely quantum effect, (i) in the antiferromagnet, the value of the specific heat peak is insensitive to anisotropy and the temperature of the specific heat peak decreases from the isotropic (Heisenberg) with introduction of either type (Ising or XY) anisotropy; (ii) in complete contrast, in the ferromagnet, the value and temperature of the specific heat peak increase with either type of anisotropy.

Excitation spectrum gap and spin-wave stiffness of XXZ Heisenberg chains: Global renormalization-group calculation

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4:06PM L27.00009 Excitation Spectrum Gap and Spin-Wave Stiffness of XXZ Heisenberg Chains: Global Renormalization-Group Calculation

4:18PM L27.00010 Dispersive excitations in the $S = 1$ antiferromagnet $Ba_3MnO_6$

We study the full Raman intensity for the Heisenberg $S = 1/2$ antiferromagnet on the triangular lattice by simultaneously considering the effects of the renormalization of the spectrum by $1/S$ correlations, and the final state magnon-magnon interactions. The analysis of the Raman intensity without final state interactions shows, that it has two peaks, corresponding to two maxima of the bare magnon spectrum $E_k$. Then we calculate Raman intensity with the renormalized spectrum. We obtain that at the energy at which the renormalized dispersion has a plateau, and, therefore, density of states is large, the Raman intensity is strongly enhanced. We also derive explicit expressions for the vertex functions of order $1/S$, and calculate Raman intensity including $1/S$ self-energy and the vertex corrections on equal footing. The vertex corrections is calculated by a summation of ladder diagrams with magnon-magnon interactions. Once interactions are included, the peak smears out and shifts to lower energies.

4:30PM L27.00011 Field dependence study on the ordering temperature of $[Cu(pz)_2(NO_3)](PF_6)$

Field dependence study on the ordering temperature of $[Cu(pz)_2(NO_3)](PF_6)$

Field dependence study on the ordering temperature of $[Cu(pz)_2(NO_3)](PF_6)$

4:42PM L27.00012 Raman scattering for the Heisenberg $S=1/2$ antiferromagnet

Raman scattering for the Heisenberg $S=1/2$ antiferromagnet

Raman scattering for the Heisenberg $S=1/2$ antiferromagnet

4:54PM L27.00013 Central peak problem in the 2d anisotropic heisenberg model

Central peak problem in the 2d anisotropic heisenberg model

Central peak problem in the 2d anisotropic heisenberg model

We acknowledge financial support from CNPq and FAPEMIG.
techniques have the potential for enabling quantum computing applications such as coupling several qubits via a quantum bus interactions in circuit quantum electrodynamics (QED) experiments \[1\].

We have used the stochastic series expansion quantum Monte Carlo method \[1\] and used the results to interpret our experimental data. For example, copper pyrazine diazide, CuPz(N\(_2\)), has a primary exchange of 15.5 K and an anisotropy parameter \(\alpha = 0.4\). The stronger exchange is due to the superexchange pathway through the pyrazine molecule and the weaker corresponds to the azide bridges. \[1\] A. Sandvik, PRB 59, R14157 (1999).

### 5:18PM L27.00015 Magnetic and Thermal Properties of the Spin \(S = 1/2\) Zig-Zag Spin Chain Compound In\(_2\)VO\(_5\) \(*\). YOGESH SINGH, DAVID JOHNSTON, Ames Laboratory — The structure of In\(_2\)VO\(_5\) consists of zig-zag V\(^{4+}\) (spin \(S = 1/2\)) chains along the \(b\)-axis. Prior to our work, there were two theoretical reports on this material.\[1,2\] One report suggested that the nearest-neighbor and next-nearest-neighbor interactions between the V\(^{4+}\) moments would be anti-ferromagnetic and frustrated,\[1\] while the second report suggested that both these interactions should be ferromagnetic.\[2\] An experimental study of the physical properties of this material had not been reported. We measured magnetic susceptibility \(\chi\), ac susceptibility \(\chi_{ac}\) and specific heat \(C\) versus temperature \(T\) on In\(_2\)VO\(_5\) and \(\chi\) and \(C\) versus \(T\) on the isostructural, nonmagnetic compound In\(_2\)TiO\(_3\). The \(\chi(T)\) data for In\(_2\)VO\(_5\) showed that the dominant magnetic exchange between the V\(^{4+}\) moments was ferromagnetic above 150 K. However, the \(\chi(T)\) and the frequency dependence of the \(\chi_{ac}(T)\) data indicate that below 3 K the system is in a spin-glass state indicating the presence of disorder and frustrated interactions at these temperatures. Our \(C\) and entropy \(S\) data suggest that there may be a structural change below 140 K in In\(_2\)VO\(_5\) which could possibly change the interactions between the V\(^{4+}\) moments.


**Tuesday, March 11, 2008 2:30PM - 5:30PM – Session L28 DCMP: Material Issues for Superconducting Qubits** Morial Convention Center 220

### 2:30PM L28.00001 Fabrication and Characterisation of Superconducting Coplanar Waveguide Resonators for Circuit QED Applications. MARTIN GÖPPLE, Department of Physics, ETH Zurich, ROB SCHOELKOPF, Department of Applied Physics and Physics, Yale University, ANDREAS WALLRAFF, Department of Physics, ETH Zurich, ETH QUANTUM DEVICE TEAM, YALE CIRCUIT QED TEAM — Superconducting thin film microwave cavities have gained great interest in recent years for studying qubit-photon or qubit-photon-qubit interactions in circuit quantum electrodynamics (QED) experiments \[1,2\]. Thin film cavities made by using standard optical lithography and microfabrication techniques have the potential for enabling quantum computing applications such as coupling several qubits via a quantum bus \[2\]. In order to specifically design circuit QED systems the cavity parameters such as resonance frequency and quality factor, determined by the input and output coupling strength need to be precisely controlled. We have fabricated niobium and aluminum resonators on Si, Si/SiO\(_2\) and Al\(_2\)O\(_3\) substrates. Resonators with quality factors up to several hundred thousands have been characterized. Furthermore, the effect of external parameters such as temperature and drive power have been investigated. The measured frequency dependent transmission of the cavities is found to be in good agreement with analytical circuit models.

1. Supported by the USDOE under Contract No. DE-AC02-07CH11358.

### 2:42PM L28.00002 Materials for superconducting qubits: Measurements of dielectric loss at low temperatures. AARON O’CONNELL, M. ANSMANN, R.C. BIALCZAK, R. MCDERMOTT, M. HOFHEINZ, N. KATZ, E. LUCERO, M. NEELEY, H. WANG, E.M. WEIG, J.M. MARTINIS, A.N. CLELAND, UC Santa Barbara — The energy relaxation time \(T_1\) of the Josephson phase qubit is significantly impacted by the microwave loss in the dielectric materials used in fabrication. This loss mechanism is most likely due to the qubit coupling to a ferromagnetic bath of two-level defect states embedded in the dielectrics. At high temperatures or high excitation voltages, these states can become saturated, so that the low loss tangents reported in the literature do not accurately represent the material performance at low temperatures and very small excitation energies. We have probed the microwave (\(~\)6 GHz) loss tangents of a number of common thin-film dielectrics at \(~\)100mK, using very low excitation voltages, in order to obtain values for the loss tangents relevant to quantum computation. We present these loss tangent data, and illustrate a technique to extract material values from measurements of the quality factors of coplanar waveguide resonators.

### 2:54PM L28.00003 Multi-level Spectroscopy of Microstates Coupled to a dc SQUID Phase Qubit. TOM VALLEAU, ROB BUTCHER, BRIAN KEITH, CHRISTOPHER LANDEE, MARK TURNBULL, Clark University, ANDERS SANDVIK, Boston University — Rectangular antiferromagnets are two-dimensional systems with inequivalent exchange strengths \((J', J)\) along the two principle axes with \(J' > J\). Our results are consistent with experimental conclusions that the critical flux \(J_c\) is much larger than the critical flux \(J_c\) for a one-dimensional system. For example, compound VO\(_2\) is frustrated at high temperatures, while the second report suggested that both \(J\) and \(J'\) are frustrated.

\[1\] A. Sandvik, PRB 59, R14157 (1999).

**3:06PM L28.00004 Effect of Two Level System Saturation on Charge Noise in Josephson Junction Quibts. MAGDALENA CONSTANTIN, CLARE YU, University of California, Irvine, JOHN MARTINIS, University of California, Santa Barbara — It is not widely appreciated that two-level systems in small qubits can easily be strongly saturated when the applied electromagnetic flux \(J\) is much larger than the critical flux \(J_c\). We show that charge noise \(S_Q\) in Josephson qubits can be produced by fluctuating two-level systems with electric dipole moments in the substrate using the standard flat density of states. At high frequencies the frequency and temperature behavior of the charge noise depends on the ratio \(J_c/J_d\). Our results are consistent with experimental conclusions that \(S_Q \sim 1/f\) at low frequencies and \(S_Q \sim f\) at high frequencies.
3:18PM L28.00005 Crystalline Josephson phase qubits with improved performance. JEFFREY KLINE, SEONGSHIK OH, National Institute of Standards and Technology. HAOHUA WANG, JOHN MARTINIS, U.C. Santa Barbara, DAVID PAPPAS, National Institute of Standards and Technology — One of the greatest challenges in the development of a practical solid-state quantum computer is to overcome decoherence due to coupling between the environment and the qubit. Superconducting quantum computers based on Josephson phase qubits are susceptible to decoherence due to charge noise in both the tunnel barrier and crossover insulators. We have demonstrated that the usage of crystalline tunnel barriers greatly reduce the density of spurious charge fluctuators in the tunnel barrier when compared to the ubiquitous amorphous barrier. However, a performance gain in coherence time was not realized due to decoherence in the crossover insulator. In the latest generation of devices, we have optimized both the tunnel barrier and crossover insulator materials. Low temperature measurements performed on a large area (50 μm²) device yielded a coherence time of 500 ns which is tied for the Josephson phase qubit world record. We expect increased performance in future generation devices where small area (13 μm²) junctions will be used.

3:30PM L28.00006 1/f Flux Noise in Josephson Phase Qubits1, ROBERT MCDERMOTT, UW-Madison Dept. of Physics, RADEK BIALCZAK, MÁRKUS ANSMANN, MAX HOFHEINZ, NADAV KATZ, ERIK LUCERO, MATTHEW NEELEY, AARON O’CONNELL, HAOHUA WANG, ANDREW CLELAND, JOHN MARTINIS, UCSB Dept. of Physics — We present the results of a novel measurement in a Josephson phase qubit which uses the resonant response of the qubit to directly measure the spectrum of low-frequency noise. This general method can be applied to any qubit system. By alternating the sense of the qubit bias, we show that the noise is predominantly flux-like, as opposed to a critical-current noise. The magnitude of the noise is compatible with previous measurements of excess low-frequency flux noise in SQUIDs cooled to millikelvin temperatures. We present the results of calculations of flux noise from paramagnetic defects in the native oxides of the superconductors, and show that the measured flux noise cannot be explained by the standard model of two-level state defects.

3:42PM L28.00007 Measurements of Decoherence in rf SQUID Qubits1, DOUGLAS BENNETT, LUIGI LONGOBARDI, VIJAY PATEL, DMITRI AVERIN, JAMES LUKENS, Stony Brook University, Department of Physics and Astronomy — We report measurements of coherence times of an rf SQUID qubit using pulsed microwaves and rapid flux pulses. The modified rf SQUID has independent, in situ, controls for the relative positions of levels in different fluxoid wells and the barrier height between the wells. The decay of coherent oscillations is dominated by the lifetime of the excited state and low frequency flux noise. The low frequency flux noise is observed using microwave spectroscopy and resonant tunneling between fluxoid states in addition to the decay of coherent oscillations. These measurements are useful for evaluating the various insulating layers which are believed to be an important source of 1/f noise in many superconducting qubits.

3:54PM L28.00008 Josephson junction microscope for probing and quantum manipulation of low-frequency fluctuators1, LIN TIAN, Department of Applied Physics and E. L. Ginzton Laboratory, Stanford University, Stanford, CA 94305, RAYMOND SIMMONDS, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305-3328 — The high-Q harmonic oscillator mode of a Josephson junction can be used as a novel probe of spurious two-level systems (TLSs) inside the amorphous oxide tunnel barrier of the junction. In particular, we show that spectroscopic transmission measurements of the junction oscillator mode can reveal how the coupling magnitude between the junction and the TLSs varies with an external magnetic field applied in the plane of the tunnel barrier. The proposed experiments offer the possibility of clearly resolving the underlying coupling mechanism for these spurious TLSs, an important decoherence source limiting the quality of superconducting quantum devices. Meanwhile, quantum manipulation of the TLSs via the junction oscillator mode can also be achieved. L. Tian and R. W. Simmonds, Phys. Rev. Lett. 99, 137002 (2007).

4:06PM L28.00009 Low-frequency Flux Noise in SQUIDs and Superconducting Qubits, STEVEN SEnDELBACH, DAVID HOVER, ACHIM KITTEL, MICHAEL MUECK, ROBERT MCDERMOTT, UW-MADISON DEPARTMENT OF PHYSICS COLLABORATION, INSTITUT FÜR ANGEWANDTE PHYSIK, JUSTUS-LEIBIG-UNIVERSITÄT GIEBEN COLLABORATION — Superconducting qubits are a leading candidate for scalable quantum information processing. In order to realize the full potential of these qubits, it is necessary to develop a more complete understanding of the microscopic physics that governs dissipation and dephasing of the quantum state. In the case of the Josephson phase and flux qubits, the dominant dephasing mechanism is an apparent low-frequency magnetic flux noise with a 1/f spectrum. The origin of this excess noise is not understood. We report the results of SQUID measurements that explore the dependence of the excess low-frequency flux noise on SQUID inductance, geometry, materials, and temperature. We discuss contributions to the measured noise from temperature fluctuations, trapped vortices in the superconducting films, and surface magnetic states in the native oxides of the superconductors. We discuss implications of our measurements for qubit dephasing.

4:18PM L28.00010 Small shadow evaporated junctions for superconducting phase qubits, F. ALTOMARE, M.S. ALLMAN, K. CICAK, M.A. SILLANPÄÄ1, J.D. WHITTAKER, R.W. SIMMONDS, National Institute of Standards and Technology, Boulder, CO 80305 USA — One of the biggest problems facing the fabrication of quantum computers based on superconducting qubits is the short coherence time of the quantum states. This is due to interaction of qubits with both the environment and defects (two level systems-TLS) in the Josephson junction (JJ). Because of the large JJ area, this problem is particularly obvious in phase qubits where it has been shown that TLS greatly affect the coherence time. One way to overcome this problem is to reduce the size of the JJ thus reducing the number of TLS. We will discuss the results of our approach to this solution, namely using shadow evaporated JJ (< 1μm²) and low-loss capacitor, and the results of our experiments on coupled qubits.

4:30PM L28.00011 Investigating two-level systems in the Josephson tunnel barrier1, JOSHUA STRONG, NIST, FABIO ALTOMARE, RAYMOND SIMMONDS — The presence of two-level system defects within the Josephson tunnel barrier has been made apparent in the spectroscopy of superconducting phase quantum bits. Here, we present a different circuit—a tunable harmonic resonator based on the Josephson inductance— which is better suited to the study of these two-level systems. A typical circuit is tunable over a gigahertz range and behaves linearly at sufficiently low drive amplitudes. We use this circuit to investigate the properties of individual defects, extracting parameters such as strength of coupling to the resonator, etc. The sea of two-level systems also has a bulk effect, causing a degradation in the quality factor of the resonator. This means that the Josephson tunnel barrier has a non-zero loss tangent in the microwave regime.

1Supported by DTO under Grant No. W911NF-05-R-0009.
2This work has been supported in part by NSF and by AFOSR and NSA through a DURINT program.
3L. T. is supported by the SORST of JST and the Karel Urbanek Fellowship; R.W. S. is supported by NIST and DTO under Grant No. W911NF-05-R-0009.
4Current Address: Helsinki University of Technology, Low Temperature Laboratory, Finland
5PRL 93, 077003 (2004)
6PRL 97, 050502 (2006)
4:42PM L28.00012 Probing dissipation from vortices with superconducting microwave resonators. C. SONG, T.W. HEITMANN, M.P. DEFOE, K. YU, B.L.T. PLOURDE, Syracuse University; R. MCDERMOTT, University of Wisconsin — One potential source of dissipation in superconducting films comes from vortices trapped in the thin films. We present a design for a system of microwave resonators for studying the loss contributed by trapped flux over the frequency range from 2 - 12 GHz. This consists of a multiplexed set of superconducting resonators with a wide range of lengths that are capacitively coupled to a common superconducting feed-line. By cooling the resonators in different magnetic fields, it is possible to probe the loss from vortices as a function of field and frequency, at least at the discrete frequencies of the resonators in our set.

4:54PM L28.00013 Decoherence in Superconducting Qubits from Surface Magnetic States, DAVID HOVER, STEVEN Sendelbach, UW-Madison Department of Physics, ACHIM KITTEL, Institut für Angewandte Physik, MICHAEL MUECK, Justus-Leibig-Universität Gießen, ROBERT MCDERMOTT, UW-Madison Department of Physics, UW-MADISON DEPARTMENT OF PHYSICS COLLABORATION, INSTITUT FÜR ANGEWANDTE PHYSIK COLLABORATION, JUSTUS-LEIBIG-UNIVERSITÄT GIEBEN COLLABORATION — Unpaired spins in amorphous surface oxides can act as a source of decoherence in superconducting and other solid-state qubits. A density of surface spins can give rise to low-frequency magnetic flux noise, which in turn leads to dephasing of the qubit state. In addition, magnetic surface states can couple to high-frequency resonant magnetic fields, and thereby contribute to energy relaxation of the qubit. We present the results of low-frequency measurements of the nonlinear and imaginary spin susceptibility of surface magnetic states in superconducting devices at millikelvin temperatures. In addition, we describe high-frequency magnetic resonance measurements that directly probe the surface spin density of states. We present calculations that connect the measurement results to qubit energy relaxation and dephasing times.

5:06PM L28.00014 Measurement of low frequency flux noise in superconducting flux qubits1. WEI QIU, BO MAO, Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, YANG YU, Department of Physics, Nanjing University, Nanjing 210093, China, SHAOXIONG LI, SIYUAN HAN, Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, DEPARTMENT OF ELECTRONICS SCIENCE AND ENGINEERING, NANJING UNIVERSITY COLLABORATION — The development of superconducting quantum interference device (SQUID) technology has been impeded significantly in the last several years by excessive low frequency flux noise which has become the dominant decoherence mechanism in several experiments. We measured the low frequency flux noise in SQUIDs with inductance ranging from about 30 pH to 1 nH. We found that for the Nb SQUIDs fabricated with the same process the measured rms low frequency flux noise has a linear dependence on the inductance of the SQUIDs. Implications of the result on material, design, fabrication of flux qubit will be discussed.

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1This work was supported in part by NSF Grant No. DMR-0325551.

5:18PM L28.00015 Measurement of Spin Susceptibility of Thin Films and Nano-Scale Structures, JULIE BERT, HENDRIK BLUHM, NICHOLAS KOSHNICK, Stanford University; MARTIN HUBER, University of Colorado Denver, KATHRYN MOLER, Stanford University — We report measurements of a spin-like paramagnetic susceptibility signal from high purity metallic and insulating thin films. The measurements were performed using a Superconducting Quantum Interference Device (SQUID) in a scanning microscope. By using the SQUID to scan areas of the sample both near and far from the metallic films, we found a paramagnetic susceptibility associated with both Au and AlOx films that was ten times larger than could be explained by the concentration of impurity spins expected for 6N gold. The 1/T temperature dependence and the paramagnetic sign indicate that the susceptibility signal is caused by localized spins that are at most weakly coupled to each other and to the conduction electrons. Moreover, the signal exhibits a measurable out of phase response which can be related to 1/f noise due to fluctuating spins [Koch, Divincenzo, and Clarke, Phys. Rev. Lett. 98, 267003 (2007)]. These results demonstrate the utility of scanning SQUID based susceptibility measurements for characterizing spin related effects. Further applications of this technique may include probing 1/f noise origins in superconducting devices as well as imaging magnetic structures such as nanomagnets.

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Tuesday, March 11, 2008 2:30PM - 5:30PM —

Session L29 DMP: Focus Session: Carbon Nanotubes and Related Materials VIII: Electronic Structure of Graphene, Morial Convention Center 221

2:30PM L29.00001 Electronic Structure and Morphology of Graphene Layers on SiC, TAI SUKE OHTA, Lawrence Berkeley National Laboratory/Fritz Haber Institute — Recent years have witnessed the discovery and the unique electronic properties of graphene, a sheet of carbon atoms arranged in a honeycomb lattice. The unique linear dispersion relation of charge carriers near the Fermi level ("Dirac fermions") lead to exciting transport properties, such as an unusual quantum Hall effect, and have aroused scientific and technological interests. On the way towards graphene-based electronics, a knowledge of the electronic band structure and the morphology of epitaxial graphene films on silicon carbide substrates is imperative. We have studied the evolution of the occupied band structure and the morphology of graphene layers on silicon carbide by systematically increasing the layer thickness. Using angle-resolved photoemission spectroscopy (ARPES), we examine this unique 2D system in its development from single layer to multilayers, by characteristic changes in the π band, the highest occupied state, and the dispersion relation in the out-of-plane electron wave vector in particular. The evolution of the film morphology is evaluated by the combination of low-energy electron microscopy and ARPES. By exploiting the sensitivity of graphene’s electronic states to the charge carrier concentration, changes in the on-site Coulomb potential leading to a change of π and π* bands can be examined using ARPES. We demonstrate that, in a graphene bilayer, the gap between π and π* bands can be controlled by selectively adjusting relative carrier concentrations, which suggests a possible application of the graphene bilayer for switching functions in electronic devices. This work was done in collaboration with A. Bostwick, J. L. McChesney, and E. Rotenberg at Advanced Light Source, Lawrence Berkeley National Laboratory, K. Horn at Fritz-Haber-Institut, K. V. Emteev and Th. Seyller at Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, and F. El Gabaly and A. K. Schmidt at National Center for Electron Microscopy, Lawrence Berkeley National Laboratory.

3:06PM L28.00002 Tailoring electronic properties in coated graphene, BRUNOUCHOA, C.-Y. LIN, N.M.R. PERES, J.M.B. LOPES DOS SANTOS, A.H. CÁSTRO NETO, Boston University — Graphene is a single layer carbon material whose unique properties in transport are tied to its peculiar Fermi surface, which is made out of six points at the corners of the Brillouin zone where the conduction and valence bands touch. Due to the vanishing density of states at these points, the low energy excitations are made of massless Dirac fermions, with several anomalous properties in transport. We propose that some of the unique properties of graphene can be tailored by the chemical adsorption of impurity atoms on its surface. If on one hand the impurities atoms are good charge donors and can be used to control the number of charge carriers in graphene, transition metals have a more covalent character and can be used to induce magnetism. We show that despite pure graphene cannot be magnetized, the hybridization of the carbon orbitals with non-magnetic d orbitals can generate strong itinerant magneticity in graphene coated with transition metal atoms. On the other hand, if an isolated impurity atom is able to form a stable localized level under hybridization with the bath of electrons in graphene, we show that the suppression of the density of states at the localized level can strongly favor the formation of a local magnetic moment at the impurity. We propose that the local magnetization of the impurity can be controlled by the application of an external gate voltage.
WALTER DE HEER, Georgia Institute of Technology — Graphite oxide is a layered semiconducting material that is produced from graphite or graphene by LI, XIAOSONG WU, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology - USA; CNRS - Institut Neel, Grenoble - France, ∼

of several picoseconds. For bulk graphite, a decay time of using 100-fs optical pump pulses at a wavelength of 400 nm and probe pulses at a wavelength of 800 nm. We observed a transient response on the time scale

Brookhaven National Laboratory, SAMI ROSENBLATT, HUGEN YAN, JANINA MAULTZSCH , TONY HEINZ, Columbia University — The ultrafast dynamics

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For the bi-layer, a strong absorption peak was seen at 0.37eV. The absorption spectrum of tri-layer graphene was found to be well represented by the sum of those

HEINZ, Columbia University — Absorption spectra in the infrared range (0.3 – 1 eV) were measured for large-area, single-crystal mono-, bi- and tri-layer

Multi-layer Graphene Samples

 layers in the Visible and Near-Infrared

energy distribution, how they are modified by the application of external electric fields, and differences with respect to the polarity of the fields. The calculated results will be compared to the electronic and structural properties observed in scanning tunneling microscopy experiments.

Columbia University — Single-crystal mono- and multi-layer graphene samples were prepared by mechanical exfoliation on quartz substrates. The absorption spectra of samples of 1 – 3 monolayer thickness were measured in the optical and near-infrared range. The absorption coefficient was found to be largely independent of photon energy and linear in the number of graphene layers. Such absorption measurements can thus be used to determine the thickness of mesoscopic graphite to monolayer accuracy, as already demonstrated in the context of Rayleigh scattering [Casiraghi et al. Nano Letters 2007]. By analysis of the optical transmission problem for a thin film at the air-quartz interface, we deduced an absorption of 2.3% per layer. The magnitude of the monolayer absorption agrees with the value of $\pi \alpha$, where $\alpha$ is the fine-structure constant, and corresponds the result obtained from a tight-binding model of the graphene electronic structure [Gusynin et al. PRL 2006]. The predicted (and measured) optical absorption, we note, is equivalent to a constant optical conductance of $\sigma_{xx} = 6.09 \times 10^{-5} \Omega^{-1}$.

4:06PM L29.00007 Experimental Measurement of Ultrafast Carrier Dynamics in Mono- and Multi-layer Graphene Samples , DAOHUA SONG, KIN FAI MAK, YANG WU, CHUN HUNG LUI, Columbia University, MATTHEW SFEIR, Brookhaven National Laboratory, SAMI ROSENBLATT, HUGEN YAN, JANINA MAULTZSCH , TONY HEINZ, Columbia University — The ultrafast dynamics of charge carriers in mono- and multi-layer graphene was investigated by femtosecond transient reflectivity measurements. The experiments were performed using 100-fs optical pump pulses at a wavelength of 400 nm and probe pulses at a wavelength of 800 nm. We observed a transient response on the time scale of several picoseconds. For bulk graphite, a decay time of $\sim$ 3 ps was found; for thin graphene multilayer samples, a reduced decay time was observed, dropping ultimately to $\sim$ 1 ps for a single graphene layer. The reflectivity transients can be understood in terms of coupling of the photo-generated electronic excitations to optical phonons, and the subsequent loss of energy from this sub-system. The possible role of graphene interactions with the quartz substrate and the effect of the graphene electronic specific heat on the decay rate will be discussed.

4:18PM L29.00008 Exposure of Epitaxial Graphene on SiC(0001) to Atomic Hydrogen1. NATHAN GUISINGER, National Institute of Standards and Technology, GREG RUTTER, Georgia Institute of Technology, JASON CRAIN, National Institute of Standards and Technology — Graphite films on SiC exhibit coherent transport properties that suggest the potential for novel carbon-based nanoelectronics applications. Recent studies suggest that the role of the interface between single layer graphene and silicon-terminated SiC can strongly influence the electronic properties of the graphene overlay. In this study, we have exposed the graphiteized SiC to atomic hydrogen in an effort to passivate dangling bonds at the interface. We have used scanning tunneling microscopy to investigate the interface surface structure following exposure to atomic hydrogen for a range of sample temperatures. Initial results indicate that regions of clean SiC were successfully passivated with atomic hydrogen below 400 °C, while the underlying interface of the graphitized regions appear to be unchanged for all temperatures studied. The threshold temperature for passivating clean SiC suggest that the passivated dangling bonds are primarily from Si atoms that are present within the SiC surface reconstruction. Although the hydrogen does not appear to penetrate below the graphene layer, initial results suggest that it does adsorb to the graphene.

1This work was supported in part by NSF grant ECS-0404084.

4:30PM L29.00009 Characterization of Epitaxial Graphene Oxide , FAN MING, MICHAEL SPRINKLE, XUEBIN LI, XIAOSONG WU, Georgia Institute of Technology, CLAIRE BERGER, Georgia Institute of Technology - USA; CNRS - Institut Neel, Grenoble - France, WALTER DE HEER, Georgia Institute of Technology — Graphite oxide is a layered semiconducting material that is produced from graphite or graphene by chemical oxidation. The material is characterized by various probes such as transport, Raman spectroscopy and optical absorption spectroscopy. Here we present the properties of graphite oxide, which is chemically converted from epitaxial graphene directly on silicon carbide chips. The absorption spectrum indicates a large band gap and the Raman spectrum shows a pronounced D line while the 2D line is absent.
Depto de Física - UFMG — The authors introduce a geometry for ultrathin Au and Ag wires that is analyzed in terms of an interplay between geometric and electronic structure effects. Conductivity of individual graphene oxide sheets on silica/silicon substrate were measured with a 4-electrode configuration at room temperature. The conductance was found to be in the range of 500 to 1000 S/cm.

5:45PM L29.00011 Electrical conductivity of graphene oxide sheets and networks of such sheets1. Supported by the NASA through the University Research, Engineering, and Technology Institute on Bio-inspired Materials (BiMat) and by the DARPA Center on Nanoscale Science and Technology for Integrated Micro/Nano-Electromechanical Transducers (IMINT).

5:06PM L29.00012 The epitaxial graphene-graphene oxide junction, a key step towards epitaxial graphene electronics. We report on a theoretical study of the influence of electron-electron interactions on the one-particle Green’s function of a doped graphene sheet based on the random-phase-approximation and on graphene’s massless Dirac equation continuum model. We find that the presence of Schottky barriers, due to the band gap in GO, is essential to obtaining a high conductance.

5:18PM L29.00013 Plasmons and The Spectral Function of Graphene. We acknowledge support from the Brazilian agencies: FAPEMIG, CAPES, CNPq, and Instituto do Milênio de Nanotecnologia/MCT.

2:30PM L30.00001 Surface scattering in metallic nanowires. We study the dynamical motion of the atoms in the wire. Soft phonon modes were studied. It has been found that the lowest phonon states are associated with motions of atom in the middle of the chain. Atomic motion of this mode was studied by solving the nuclear wavefunction of the wire.

2:42PM L30.00002 Phonon mode and Breakdown of a Au nanowire between electrodes. We report on a theoretical study of the influence of electron-electron interactions on the one-particle Green’s function of a doped graphene sheet based on the random-phase-approximation and on graphene’s massless Dirac equation continuum model. We find that the presence of Schottky barriers, due to the band gap in GO, is essential to obtaining a high conductance.

2:54PM L30.00003 Semiconducting chains of gold and silver1. We acknowledge support from the Brazilian agencies: FAPEMIG, CAPES, CNPq, and Instituto do Milênio de Nanotecnologia/MCT.
3:06PM L30.00004 Bonding, Conductance and Magnetization of Oxygenated Au Nanowires

Chun Zhang, Robert Barnett, Uzi Landman, School of Physics, Georgia Institute of Technology — Spin-density-functional calculations of tip-suspended gold chains, with molecular oxygen, or dissociated oxygen atoms, incorporated in them, reveal structural transitions for varying lengths. The nanowires exhibit enhanced strength for both oxygen incorporation modes, and upon stretching tip atoms join the wire. With incorporated molecular oxygen the wire conductance is about 1(2e2/h), transforming to an isolating state beyond a critical length. The nanowire conductance with embedded oxygen atoms is low, 0.2 (2e2/h), and it develops magnetic moments localized on the oxygen and the neighboring Au atoms. *Physical Review Letters* (in press)

3:18PM L30.00005 ABSTRACT WITHDRAWN

3:30PM L30.00006 Superconductivity and metal-insulator transition in Bi nanowires.1

Mingliang Tian, Jian Wang, Nitesh Kumar, Qi Zhang, Thomas Malouk, Jianendra Jain, Moses H.W. Chan, Center for Nanoscience, Penn State University — Semi-metallic bismuth has long been a prototype system for quantum transport and finite-size effect studies, due to its long electron mean-free path, low carrier density and small carrier mass. We found Bi nanowires (NWs) of less than 100 nm diameter can be superconducting, metallic and insulating closely depending on the details of their microstructures, morphology and surface condition. For granular Bi NWs with grains showing (001) preferred orientation, the NWs are superconducting with Tc’s of 7.2 and 8.3 K. Without (001) preferred orientation, the NWs show superresistive behavior. For single-crystalline Bi NWs, when the wires are embedded inside anodized aluminum oxide (AAO) membrane, insulating behavior is found below 1.0 K with low excitation current but metallic at a higher bias current. However, this metallic state can be tuned into isolating again by an applied magnetic field. We have also made measurements on an individual single-crystalline Bi NWs released from the AAO, an thin oxide layer is found on the wire surface. Interestingly, the wire was found to be superconducting below 1.5 K.

1Work supported by NSF under a MRSEC grant, DMR-0213623.

3:42PM L30.00007 Evolution of Integer Quantized Conductance in Gold Nanowires.

Yoshihiko Kuriu, Dept. Cond. Matt. Physics, Tokyo Institute of Technology, Yoshifumi Oshima, Dept. Materials Science & Engineering, Tokyo Institute of Technology, Japan; Tokai University, Japan, K. Takayanagi, Mechanical Engineering Research Laboratory, Japan. — In the metallic regime, the conductance was quantized in units of the conductance quantum $G_0 = 2e^2/h$. The quantized conductance $G_n$, $n = 0, 1, 2, 3, \ldots$ was measured when the nanowires were contacted by submicron electrodes from above. By employing 4- and 2-probe configurations, not only the intrinsic electrical resistivities of the individual nanowires were measured, but also the electronic contact resistances, $R_c(T)$, have been determined. Several models are available for $R_c(T)$, including the thermal-activation model, the thermal-activation model involving three activation energies, and the thermal-activation model involving two activation energies.

3:54PM L30.00008 Intrinsic Electrical-Transport Properties of Single ZnO Nanowires.

S.P. Chiueh, Y.H. Lin, J.J. Lin, Institute of Physics, National Chiao Tung University, Taiwan, W.B. Jian, Department of Electrophysics, National Chiao Tung University, Taiwan, Z.Y. Wu, F.R. Chen, J.J. Kai, Department of Engineering and System Science, National Tsing Hua University, Taiwan. — Single-crystalline zinc oxide (ZnO) nanowires (NWs) were synthesized by the thermal evaporation method. The intrinsic electrical-transport properties of ZnO NWs were studied by carrying out four-probe measurements on individual NWs. The electrodes were made by the standard electron-beam lithography technique. The current-voltage characteristics and the zero-bias resistivities, $\rho(T)$, were measured over a wide range of temperatures between 0.25 and 300 K. We found that, in many cases, the temperature behavior of $\rho$ could be well-described by the thermal-activation model involving three activation energies ($E_1$, $E_2$, and $E_3$). Our values of $E_1$ (approximately, several tenths meV) and $E_2$ (approximately, several meV) were extracted from the $\rho(T)$ data. The $E_3$ (approximately, thousands meV) value was determined by fitting the $\rho(T)$ in the intermediate temperature regime with the thermal-activation model involving two activation energies. The $E_3$ value was found to agree well with the current understanding of the rutile material within the framework of the Boltzmann transport theory. On the other hand, we found that, for high-resistance contacts, $R_c$ increases rapidly with decreasing temperature and finally saturates at liquid-helium temperatures. This behavior of $R_c$ can be satisfactorily explained in terms of the “thermally fluctuation-induced tunneling” conduction through a microscopic junction incidentally formed at the interface between the electrode and the NW.

4:06PM L30.00009 Electrical-transport studies of individual RuO2 nanowires and their nanowire contacts.

Y.H. Lin, Institute of Physics, National Chiao Tung University, Taiwan, K.J. Lin, F.R. Chen, J.J. Kai, Department of Engineering and System Science, National Tsing Hua University, Taiwan. — Single-crystalline RuO2 nanowires (NWs) have been prepared by the thermal evaporation method. The conductance of gold junction was measured by employing a four-probe configuration. The conductance histogram exhibits the quantized conductance $G_n$, $n = 0, 1, 2, 3, \ldots$. The conductance $G_n$ was measured when the NWs were contacted by submicron electrodes from above. By employing 4- and 2-probe configurations, not only the intrinsic electrical resistivities of the individual nanowires were measured, but also the electronic contact resistances, $R_c(T)$, have been determined. Our measured resistivity behavior of the NWs is found to agree well with the current understanding of this rutile material within the framework of the Boltzmann transport theory. On the other hand, we found that, for high-resistance contacts, $R_c$ increases rapidly with decreasing temperature and finally saturates at liquid-helium temperatures. This behavior of $R_c$ can be satisfactorily explained in terms of the “thermally fluctuation-induced tunneling” conduction through a microscopic junction incidentally formed at the interface between the electrode and the NW.


Wen-Hao Wu, Hai-Dong Liu, Zuxin Ye, Zhiping Luo, K. D. D. Rathanayaka, Texas A & M University — We report an anomalous proximity effect observed in single-crystal nanowires of Zn, Sn, and Pb of length up to 60 μm. These nanowires were electrochemically deposited into the pores of anodic aluminum oxide membranes and polycarbonate membranes. Using an in situ self-contacting method, single nanowires were electrically contacted on both ends to a pair of macroscopic film electrodes of Au, Sn, and Pb. The conductance and the superconducting transition temperature were measured by employing a four-probe configuration. The conductance of the nanowires was found to be quantized in units of the conductance quantum $G_0 = 2e^2/h$. The $C_0$ and $C_1$ conductance peaks in the vicinity of $C_0(=2e^2/h)$ were observed at lower temperatures, while simultaneously acquiring transmission electron microscope images. The conductance histogram exhibits the quantized conductance $G_n$, $n = 0, 1, 2, 3, \ldots$. The conductance $G_n$ was measured when the NWs were contacted by submicron electrodes from above. By employing 4- and 2-probe configurations, not only the intrinsic electrical resistivities of the individual nanowires were measured, but also the electronic contact resistances, $R_c(T)$, have been determined. Our measured resistivity behavior of the NWs is found to agree well with the current understanding of this rutile material within the framework of the Boltzmann transport theory. On the other hand, we found that, for high-resistance contacts, $R_c$ increases rapidly with decreasing temperature and finally saturates at liquid-helium temperatures. This behavior of $R_c$ can be satisfactorily explained in terms of the “thermally fluctuation-induced tunneling” conduction through a microscopic junction incidentally formed at the interface between the electrode and the NW.

This work is supported by NSF under Grant Nos. DMR-0551813, DMR-0606529 and DMR-0315476.
4:30PM L30.00011 Electronic Transport of TiO$_2$ Nanowire Devices. Geetha Dholakia, Elore/NASA Ames Research Center, STEVEN KUO, NASA Ames Research Center, San Jose State University. Emily Allen, Dept. of Materials Engineering, San Jose State University — Titanium dioxide (TiO$_2$) is a wide band-gap semiconductor with applications in photovoltaics and sensing. Large scale integration of nanowires onto functional devices requires new techniques to manipulate them at the nanoscale. Currently engineering strategies for efficient assembly of nanoscale objects is very limited. Here we report the use of dielectrophoresis to assemble TiO$_2$ nanowires onto devices. We use a sol-gel template based synthesis of TiO$_2$ nanowires. The nanowires have a typical diameter of 100-150 nm and a length of 3-10 µm. Devices for two probe and four probe measurements were fabricated by standard lithography. AC dielectrophoresis was used to assemble the TiO$_2$ nanowires on devices. A dielectrophoretic translational force and a torque aligns the nanowires onto the devices. FIB assisted platinum deposition on the aligned TiO$_2$ nanowires ensures ohmic contacts. Two probe room temperature I-V measurements show a resistivity of 0.22 Ω-cm, which is comparable to 0.26 Ω-cm for a thin film1. Temperature dependent transport measurements are being pursued. We have demonstrated an efficient method of assembling and fabricating nanowire device structures. T. Miyata et. al. Thin Solid Films, 496, 136 (2006).

4:42PM L30.00012 Conductivity of MgZnO nanoparticles as a function of gas exposure and temperature. Chris Berven, Joseph Dick, Leah Bergman, Jesse Huso, John Morrison, University of Idaho — Changes in the current-voltage (I-V) characteristics of Mg$_{x}$Zn$_{1-x}$O ($x \approx 0.15$) nanoparticles as a function of gas exposure and temperature are reported. The nanoparticles were prepared using wet chemical techniques on insulating thermally grown SiO$_2$ substrates. We find that the photoconductivity is not sensitive to the value of the gate voltage applied to the underlying silicon, but only to changes in the energetic and spatial position of individual defects in semiconductor nanoelectronic devices.

5:06PM L30.00014 Remarkable Effects of Gating on the Photoconductivity of Porphyrin Nanorods. C. K. Riley, X. Huang, W. F. Smith, Haverford College, D. E. Johnston, A. T. Johnson, Univ. of Pennsylvania — Tetrakis(4-sulfonatophenyl) porphine self assembles into well-defined nanorods with intriguing photoelectronic properties. For example, when light is applied, the conductivity immediately jumps up from zero, then grows further over several hours. This may be due to a light-induced structural change. In recent experiments, we imaged the nanorods with AFM while measuring the photoconductivity; we observed no change in morphology. We also deposited nanorods onto oxidized silicon substrates. Contact to the nanoparticle film was made by gold wires laid across about 2 mm apart. The experiments were performed in a custom-built environmental chamber with the ability to evacuate or introduce various gases. For these experiments, the temperature was tuned over a range of about 300 K to 420 K. Our measurements showed a possible history-dependant behavior in changes of the conductance of the nanoparticle film. When the device was heated to ~120 K in vacuum or in an Ar the current increased by the same amount. When repeated with H$_2$, the current increase was less. Initially, the effect was quite pronounced with a relative change by a factor of 20. With repetitions of the experiments, the same effect was observed but to a lesser degree suggesting a saturation phenomena. When the experiment was modified so that the H$_2$ gas was introduced at a high temperature to an evacuated chamber the current dropped but not by the same degree as before. A similar response to exposure to H$_2$ was found for exposure to O$_2$. Possible explanations for the observations will be presented.

5:18PM L30.00015 Adsorption Kinetics of Alkanes on Purified HiPco Nanotubes. Dinesh Rawat, Murat Bulut, Aldo Migone, Southern Illinois University, Carbondale, IL-62901, USA — We present results for the adsorption kinetics of methane, ethane and butane on purified HiPco SWNTs. We studied the adsorption kinetics by monitoring the evolution of the gas pressure with time from the instant at which a dose of adsorbate is added to the sample, until the moment at which equilibrium is reached. The waiting times for comparable coverages increase with increasing alkane chain length. For methane and ethane, the equilibration time decreases with increasing fractional coverage. For the butane, on the other hand, the kinetic measurements display a reverse trend: the equilibration times increase with increasing fractional coverage. We speculate that this observed increase in the waiting time is due to a possible reorientation of adsorbed molecules in the film. The observed differences in adsorption kinetics suggest the possibility of using adsorption as a means to achieve the separation of gaseous alkane mixtures.

Tuesday, March 11, 2008 2:30PM - 5:30PM — Session L31 DCMP: Graphene: Atomic Structure and Lattice Properties

2:30PM L31.00001 Nano-Engineering Defect Structures on Graphene1. Mark Lusk, Lincoln Carr, Department of Physics, Colorado School of Mines — We present a new way of nano-engineering graphene using defect domains. These regions have ring structures that depart from the usual honeycomb lattice, though each carbon atom still has three nearest neighbors. A set of stable domain structures is identified using density functional theory (DFT), including blisters, ridges, ribbons, and meta-crystals. All such structures are made solely out of carbon; the smallest encompasses just 16 atoms. Blisters, ridges and meta-crystals rise up out of the sheet, while ribbons remain flat. In the vicinity of vacancies, the reaction barriers to formation are sufficiently low that such defects could be synthesized through the thermally activated restructuring of coalesced adatoms. These defect domains may offer technological applications associated with the confinement and transport of charge.

2:42PM L31.00002 Solid State Zwitterions realized on carbon graphenic surface. Zhaohui Huang, Vincent Crespi, Dept. of Physics, Penn State Univ. — Zwitterions are single molecular species that combine anionic and cationic groups. Here we consider the prospects for introducing the concept of a zwitterion into the solid state, by combining geometrically incompatible anionic and cationic moieties within a single extended structural element whose covalent rigidity frustrates the close approach of the anionic and cationic regions. Specifically, first principles computations for anionic and cationic groups such as NH$_3$ and CO$_2$ covalently attached to a graphenic surface via linker elements demonstrate long-range charge transfer, the hallmark of a zwitterion, while maintaining overall structural integrity.

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1LDC was supported by the National Science Foundation under Grant PHY-0547845 as part of the NSF Career program.
2:54PM L31.00003 Atomic structure of corrugated graphene. YOU LIN, XIANG GU, IVAN OLEYNIK, University of South Florida, CARTER WHITE, Naval Research Laboratory — Following its successful isolation, there has been intense interest in a single sheet of graphite, known as graphene, due to its fundamental physical properties as well as its promising applications in nanoelectronic devices. Recent experimental studies of graphene, freely suspended on nanofabricated scaffolding, found appreciable deviations from a perfect two-dimensional crystalline structure [1]. In this presentation, we discuss results of atomistic modeling of graphene with the occurrence of possible corrugated structures examined under the influence of several factors including sample size and temperature. [1] J.C. Meyer, et al, Nature 446, 60 (2007).

3:06PM L31.00004 Ab initio study on atomic and electronic structures of epitaxial graphene. SEUNGCHUL KIM, JISOOON IHPM, Department of Physics and Astronomy, Seoul National University, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, YOUNG-WOO SON, Department of Physics, Konkuk University — Recently, lots of efforts have been devoted to the growth of epitaxial graphene and its geometric and electronic structure measurements. Several models for the interface structure have been suggested but never been successful in explaining the observations from various experiments. Using density functional theory (DFT) calculations, we find an interface atomic structure of graphene on hexagonal silicon carbide which agrees well with the low energy electron diffraction (LEED), scanning tunneling microscopy (STM), as well as angle resolved photo emission spectroscopy (ARPES). Our results clearly resolve the disagreement between \(6 \times 6\) periodic pattern from STM measurements and the \(6\sqrt{3} \times 6\sqrt{3}\) from the LEED measurements. Furthermore, we also investigate the origin of the gap opening at the Dirac point in the present geometry.

3:18PM L31.00005 Phonon dispersions and vibrational properties of monolayer, bilayer, and trilayer graphene\(^1\). JIA-AN YAN, W. Y. RUAN, M. Y. CHOU, School of Physics, Georgia Institute of Technology, GEORGIA INSTITUTE OF TECHNOLOGY — The phonon dispersions of monolayer and few-layer graphene (AB bilayer, ABA and ABC trilayers) are investigated using the density-functional perturbation theory (DFPT). Compared with the monolayer, the optical phonon \(E_{a2g}\) mode at \(n\) splits into two and three doubly degenerate branches for bilayer and trilayer graphene, respectively, due to the weak interlayer coupling. These modes are of various mode symmetry and exhibit different sensitivity to either Raman or infrared (IR) measurements (or both), and therefore the combination of Raman and IR measurements of the zone-center optical modes should give a clear identification of the layer number as well as the stacking geometry. The splitting is found to be \(5 \text{ cm}^{-1}\) for bilayer and \(2 \text{ cm}^{-1}\) for trilayer graphene. The interlayer coupling is estimated to be about \(2 \text{ cm}^{-1}\). We found that the highest optical modes at \(K\) upshift by about \(12 \text{ cm}^{-1}\) for bilayer and \(18 \text{ cm}^{-1}\) for trilayer relative to monolayer graphene. The atomic displacements of these optical eigenmodes are analyzed.

\(^1\)This work is supported by the Department of Energy (Grant No. DE-FG02-97ER45632) and by the National Science Foundation (Grants No. DMR-02-05328).

3:30PM L31.00006 Structural study of the phase evolution of 6H-SiC(0001) by low energy electron microscopy. JIEBING SUN, KARSTEN POHL, University of New Hampshire, RUDOLF M. TROMP, JAMES B. HANNON, IBM T. J. Watson Research Center — The surface phase transition of Si-terminated 6H-SiC(0001) upon heat treatment is studied by low energy electron microscopy (LEEM). Bright and dark field imaging demonstrates a direct in situ observation of the surface phase evolution, transitions in a sequence from \(1 \times 1, 3 \times 3, \sqrt{3} \times \sqrt{3}/\sqrt{6}\) to the graphene phase due to gradually increasing the temperature. Intensity vs. voltage (IV) spectra extracted from single domain diffraction images is used to determine the local surface structure and chemical stoichiometry. Preliminary results from a quantitative dynamical analysis of the LEEM-IV curves show a Si-depleted \(1 \times 1\) structure and an adatom-trimer-adlayer structure on \(3 \times 3\) reconstruction. Ongoing work on the structure of the \(\sqrt{3} \times \sqrt{3}/\sqrt{6}\) and \(6 \times 6\) phases is aimed to unraveling the initial growth mechanism of graphene on SiC.

3:42PM L31.00007 The Initiation of Graphene Growth on SiC(0001)-6H. JAMES HANNON, RUDOLF TROMP, IBM Research Division — We have studied the evolution of surface morphology on SiC(0001)-6H during annealing at temperatures up to 1250 C using low-energy electron microscopy (LEEM). Surface roughness is dominated by the formation of deep pits or canyons. We show that the canyons form because of the stability of the \(6 \times 6\) phase, which pins atomic steps during the decomposition of SiC. The density of pits is ultimately determined by how the \(6 \times 6\) phase nucleates. Graphene forms preferentially in these pits, where the step density is highest.

3:54PM L31.00008 Imaging the interface states of epitaxial graphene layers on 6H-SiC. G. SUN, Y. QI, M. WEINERT, L. LI — Single and bi-layer graphene were epitaxially grown on both the Si- and C-terminations of 6H-SiC. The energy dependence and spatial distribution of their local density of states were investigated using scanning tunneling microscopy and spectroscopy. Of particular interest is the r\(3\)x\(3\) reconstructed interface state. Atomically resolved topographs and dI/dV images show clear differences between the single and bi-layer graphene at different length scales. These results will be compared to the electronic and structural properties obtained by first principles calculations.

4:06PM L31.00009 Interface Studies of Graphene layers on SiC thin films and bulk SiC(0001). ANNA SANDIN, J.L. TEDESCO, NC State University, R.J. NEMANICH, Arizona State University, J.E. MILLAN, J. HASS, Georgia Institute of Technology, F. VARCHON, Institut Neel/CNRS, W.A. DEHEER, C. BERGER, P.N. FIRST, Georgia Institute of Technology, L. MAGAUD, Institut Neel/CNRS, E.H. CONRAD, Georgia Institute of Technology — We present x-ray diffraction experiments showing that multilayer graphene grown on 4H-SiC(0001) (C-face) consists of a high density of rotational stacking faults. The existence of these faults explains why multilayer graphene is electronically similar to an isolated graphene sheet [1]. The faults present themselves as graphite rods rotated through a series of commensurate graphene/SiC angles relative to the SiC rods and as rods shifted due to compressed graphene at the fault boundaries. By analyzing the intensity modulations of these different rods, it is possible to extract information on the distributions of these faults in the film. We will present results from calculations of different models for the fault distribution and compare them against x-ray data for graphene films of different thicknesses. [1] J. Hass, F. Varchon, J. E. Millan-Otoya, M. Sprinkle, W.A.de Heer, C. Berger, P.N. First, L. Magaud, E.H. Conrad (to be published) http://arxiv.org/abs/0706.2134.
4:30PM L31.00011 Dispersive Raman Scattering from $n=1$-4 Graphene Layers (nGLs)  
Peter Eklund, Pennsylvania State University, Awnish Gupta, PSU — We present new Raman scattering results from nGLs ($n=1, 2, 3, 4$) in the range of 100 - 4500 cm$^{-1}$. Dispersive behavior of Raman peaks was probed at room temperature with 7 laser lines from 1.5-2.7 eV. In addition to the five Raman peaks reported previously, we report on the behavior of five new weaker features that appear in graphene (514.5 nm excitation) at $\sim$1882 cm$^{-1}$($\sim$125 cm$^{-1}$/eV), $\sim$2035 cm$^{-1}$($\sim$177 cm$^{-1}$/eV), $\sim$2218 cm$^{-1}$($\sim$43 cm$^{-1}$/eV), $\sim$3174 cm$^{-1}$($\sim$40 cm$^{-1}$/eV) and $\sim$4069 cm$^{-1}$($\sim$35 cm$^{-1}$/eV). The value in ( ) is the respective band dispersion, or shift with peak position per eV change in the excitation energy. The band dispersion is connected with the ratio of the phonon to Fermi velocity and stems from the double resonance (DR) scattering. New Raman bands that are only observed for nGLs ($n > 1$) are found at $\sim$1510 cm$^{-1}$($\sim$16 cm$^{-1}$/eV) and 1737 cm$^{-1}$ ($\sim$10 cm$^{-1}$/eV). The identities of the new peaks will be discussed based on DR scattering and the phonon dispersion curve of graphene.

4:42PM L31.00012 The Thickness Dependence of the Graphene Oxidation  
Liu Liu, Sunmin Ryu, NSEC & Department of Chemistry, Columbia University, Michelle Tomask, NSEC, Columbia University, Elena Stolyarova, Michael Steigerwald, NSEC & Department of Chemistry, Columbia University, Mark Hysbertsen, Center for Functional Nanomaterials, Brookhaven National Laboratory, Louis Brus, George Flynn$^1$, NSEC & Department of Chemistry, Columbia University — Single-, double-, and triple-layer graphene sheets were heated in an oxygen atmosphere at various temperatures generating nano-sized holes in the sheets. Both AFM topography and Raman spectroscopy indicate that the oxidative reactivity of single-layer sheets is greater than that of thicker sheets. The distribution of hole sizes and STM topography studies suggest that the oxidation reaction is initiated at the pristine carbon surface. Vertical etching of carbon atoms from the graphene surface occurred at a much lower temperature than that from a highly oriented, multi-layer pyrolytic graphite crystal. The mechanism for this thickness dependence of reactivity will be discussed.

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4:54PM L31.00013 UHV STM/STS and AFM study of oxidized graphene sheets  
Deepak Pandey, Birck Nano Technology Center, Purdue University, Richard Piner. The University of Texas at Austin, Ronald Reifenberger, Birck Nano Technology Center, Purdue University — Exfoliated oxidized graphene sheets, suspended in an aqueous solution, were deposited on freshly cleaned HOPG and studied by ambient AFM and UHV STM. The AFM images revealed oxidized graphene sheets with a lateral dimension of $\sim$5-10 µm. The oxidized graphene sheets exhibited different thicknesses and were found to conformally coat the HOPG substrate. Wrinkles and folds induced by the deposition process were clearly observed. Phase imaging and lateral force microscopy showed distinct contrast between the oxidized graphene and the underlying HOPG substrate. The UHV STM studies of oxidized graphene revealed atomic scale periodicity showing a 0.26 nm x 0.42 nm unit cell over small areas. This periodicity is identified with oxygen atoms bound to the oxidized graphene sheet. I(V) data were taken from oxidized graphene sheets and compared to similar data obtained from bulk HOPG. The dI/dV data from oxidized graphene reveals a reduced density of electron states within ±0.1 V around zero bias.

5:06PM L31.00014 Scanning Tunneling Spectroscopy (STS) studies of graphene films on an insulating substrate  
Elena Stolyarova, Li Liu, Columbia University, Mark Hysbertsen, Brookhaven National Laboratory, Philip Kim, Tony Heinz, George Flynn, Columbia University, Center for Functional Nanomaterials, BNL Team, Center for Electron Transport in Molecular Nanostructures, Columbia University Team, Department of Chemistry, Columbia University Team — Scanning Tunneling Spectroscopy has been utilized to study the differences between the electronic structure of a three-dimensional graphite crystal and its two-dimensional building block, graphene. Single and few-layer graphene samples were isolated on a non-conductive silicon dioxide substrate and contacted at the edges with a gold electrode. For single layer flakes current-voltage dependent I(V) curves, recorded at 4.6 K under Ultra-high Vacuum (UHV) conditions, show no additional features for states far from the Fermi energy that might be considered characteristic of a weak interaction between graphene and the substrate. No significant spatial inhomogeneity of local sample properties was observed. Evolution of spectroscopic curves as a function of graphene layers will be discussed.

5:18PM L31.00015 Generation of atomic scale defects in graphene by high-energy positive-ion bombardment  
Danail Stolyarov, Brookhaven National Laboratory, Elena Stolyarova, George Flynn, Columbia University, Karl Kusche, Igor Pavlishin, Igor Poporelsky, Brookhaven National Laboratory, Peter Shkolkovskii, Stony Brook University, Vitaly Yakimenko, Brookhaven National Laboratory — We have demonstrated controllable defect generation in graphene (a single layer of a graphite crystal) and in few atomic layer thick graphite films. Graphene flakes deposited on a silicon dioxide substrate by mechanical exfoliation were bombarded by a collimated high-energy (1 MeV) particle beam consisting of protons and positively charged ions. This beam was produced by Target Normal Sheath Acceleration (TNSA) upon irradiation of a metal foil with a terawatt CO2 laser pulse. Ions and protons with different mass and energy were separated by a permanent magnet installed between the laser target and the sample. After the exposure the graphene flakes were examined by Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM). Irradiation of graphene films with both protons and positive ions results in the formation of atomic-scale defects without mesoscopic damage to the film. The density of observed defects depends strongly on the number of atomic layers. This method can be used to modify single chemical bonds in graphene films and to engineer carbon based devices and sensors with tailored properties.

Tuesday, March 11, 2008 2:30PM - 5:30PM –
Session L32 GMAG DMP FLAP: Focus Session: Spin Transfer Torque II
Morial Convention Center 225

2:30PM L32.00001 Time-Resolved X-ray Microscopy for Direct Observation of Spin-Torque and Oersted-Field Driven Vortex Gyration  
M. Bolte, G. Meier, L. Bocklage, A. Drews, B. Krueger, University of Hamburg, Germany, T. Tyliszczak, ALS, LBL, Berkeley, CA, A. Vansteenkiste, B. Van Waeyenberge, Ghent University, Belgium, K.-W. Chou, H. Stoll, Max-Planck-Institute for Metal Research, Stuttgart, Germany — Due to their symmetry, magnetic vortices are ideal candidates for studying the influence of the spin-transfer torque on the local magnetization. The out-of-plane magnetization with a laser induced azimuthal chirality a chirality-dependent phase shift of $\phi_0$ is observed that is attributed to Oersted fields from the spin-polarized current. An analytical model estimates corresponding field strengths of $\mu_0 H \sim 10^{-10}$ A/m. This study confirms our assumption that Oersted fields from spin-polarized currents cannot be neglected in spin-torque experiments and shows the sensitivity of the measurement technique.
2:42PM L32.00002 Time-resolved X-ray Imaging of Spin-Torque-Induced Vortex Oscillation

XIAOWEI YU, Stanford University, VLAD PRIBIAG, Cornell University, YVES ACREMANN, Stanford Synchrotron Radiation Laboratory, VENKATESH CHEMBROLOU, Stanford University, ASHWIN TULAPURKAR, Stanford Synchrotron Radiation Laboratory, TOLEK TYLISZCZAK, Advanced Light Source, ZHIPAN LI, ROBERT BUHRMAN, Cornell University, JOACHIM STOHR, Stanford Synchrotron Radiation Laboratory, HANS SIEGMANN, PULSE Center, Stanford Linear Accelerator Center — Recent transport measurements demonstrated a persistent oscillation of a magnetic vortex isolated in a nanoscale spin-valve structure driven by STT. This vortex precession is inferred from the giant magnetoresistance (GMR) signal, which depends on the relative average magnetization of the two magnetic layers. Here, we report spatially resolved measurements of the vortex oscillation driven by spin-transfer torque by using advanced x-ray imaging technique. The microwave-frequency vortex oscillation is synchronized to the fast x-ray pulses. Motion images with 70ps time resolution and 30nm spatial resolution reveal the complicated dynamics underlying the previously observed oscillating GMR signal. [1] V. S. Pribiag, I. N. Krivorotov, G. D. Fuchs, P. M. Braganca, O. Ozatay, J. C. Sankey, D. C. Ralph, and R. A. Buhrman, Nature Physics 3, 498 (2007)

2:54PM L32.00003 Spin-current induced magnetic excitations in single magnetic layer nanopillars1

BERND BESCHOTEN, NICOLAS MÜSCENS, MARK WEIDENBACH, EVA MAYNICKE, COEN SMITS, II. Physikalisches Institut, RWTH Aachen, MATTHIAS BÜCKINS, JOACHIM MAYER, Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen, GERNOT GÜNTHERODT, II. Physikalisches Institut, RWTH Aachen — We investigate current-induced spin-wave excitations in Cu/Co/Cu single magnetic layer nanopillars with asymmetric Cu leads by means of transport and microwave probes at room temperature. The thin film stack is deposited by MBE in prefabricated nanostencil masks with lateral dimensions below 100 nm. At high current densities, we observe narrow excitations (bandwidth ~ 100 MHz) and higher harmonics for magnetic fields perpendicular to the layers. The frequency increases with increasing current and magnetic field, which indicates an out-of-plane precessional mode as found in bilayer systems (e.g., Kiselev et al., PRL 93, 036601(2004)). Furthermore, we observe frequency jumps as a function of both current and magnetic field, which might originate from transitions between different localized nonlinear spin-wave modes.

3:06PM L32.00004 Large angle out of plane steady precession induced by spin-transfer with perpendicular to plane polarizer. Dimtri Houssameddine, Spintec - CE/A/CNRS — The dynamics of a ferromagnetic system is characterized by a conservative precession torque, as well as a non-conservative damping torque. The damping torque is responsible for the realignment of the magnetization with the equilibrium direction after excitation. Recently, it has been shown that the damping torque can be compensated by a spin transfer torque that is due to the interaction between a spin polarized current and the local magnetization. This additional spin transfer torque can lead to auto-oscillations of the magnetization close to constant energy trajectories. The potential exploitation of such large angle auto-oscillations for tunable microwave devices is currently driving many research efforts. For an in-plane magnetized thin film with uniaxial anisotropy, two types of constant energy trajectories exist which are commonly called in-plane precession (IPP), where the magnetization oscillates around the in-plane energy minimum, and out of plane precession (OPP) where the magnetization oscillates around the out of plane energy maximum [1]. IPP and OPP oscillations differ substantially in their dependence of frequency and amplitude as a function of current and/or applied bias field. In many experiments so far, IPP precessions have been obtained at the threshold current using in-plane magnetized spin valve structures. However, from an applications point of view it will be of interest to excite OPP oscillations since they will lead to a larger output signal than IPP oscillations. Here, we will present experimental evidence of large angle OPP oscillations using a spin torque oscillator that contains a perpendicularly magnetized polarizing layer and an in-plane magnetized analyzing layer in addition to a planar free layer [2]. We will show that OPP oscillations are induced at the threshold current for moderate current densities of 9*10^7 A/cm^2. The experimental current-field state diagram as well as the dependence of the frequency vs. current and applied bias field is in good qualitative agreement with macrospin and micromagnetic simulations. Furthermore, due to the perpendicular nature of OPP oscillations, they allow a direct comparison of the OPP and IPP precession amplitudes. [1] A. N. Slavin, V. S. Tyberkevich Phys. Rev. B 72, 94428 (2005) [2] Houssameddine et al, Nature Materials 6, 441 (2007)

3:42PM L32.00005 Current-Induced Magnetization Switching with a Spin-Polarized Scanning Tunneling Microscope. MATTHIAS BODE, Argonne National Laboratory, STEFAN KRAUSE, University of Hamburg, LUIS BERBIL-BAUTISTA, University of California at Berkeley, GABRIELA HERZOG, WOLFGANG GUNTHERODT, University of Hamburg — The understanding of current-induced magnetization switching is in the focus of many ongoing investigations since switching the magnetization by the injection of a spin-polarized current rather than by magnetic fields may open the gateway for new data storage technologies at much higher bit densities. We show how individual superparamagnetic Fe nanoislands with typical sizes of 100 atoms can be addressed and locally switched using a magnetic scanning probe tip. We demonstrate current-induced magnetization reversal across a vacuum barrier and combine it with the ultimate resolution of spin-polarized tunneling microscopy. This technique allows us to control the nanoscale distance and quantity three fundamental contributions that are involved in magnetization switching, i.e. current-induced spin torque, heating the island by the tunneling current, and Oersted field effects.

3:54PM L32.00006 Current-Induced Magnetoresistance in Antiferromagnetic Spin Valves1

WEI, University of Texas at Austin, A. SHARMA, J. BASS, Michigan State University, M. TSOI, University of Texas at Austin — Influence of the magnetic state of a ferromagnet (F) on its electronic transport properties has been found in various phenomena, including giant magnetoresistance (GMR) in magnetic multilayers, where the relative orientation of the magnetic moments of F-layers affects the current flow. MacDonald and co-workers recently predicted that a corresponding effect - antiferromagnetic GMR (AGMR) - should exist in structures where F-layers are replaced by antiferromagnets (AFM). To test this prediction, we measured the (closely) current-perpendicular to plane (CPP) magnetoresistance (MR) of three types of AFM spin-valve multilayers: (I) AFM/N/AFM, (II) F/AFM/N/AFM, and (III) F/AFM/N/AFM/F, with a non-magnetic (N) layer between the two AFM layers. We saw no MR in samples of type I or II at any current density j, or of type III when j was small. But large enough j ~ 10^3 A/m^2 applied to type III multilayers gave small positive MRs (largest resistance at high field). As these MRs are inverted from the usual GMR of the F-layers, they must be due to the AFM layers, and thus be an AGMR. We will describe how this AGMR varied with applied current j and AFM layer thickness [arXiv:0711.0059].

4:06PM L32.00007 RF Assisted Spin Transfer Switching in Nanopillar Spin-Valves. S.H. FLOREZ, J.A. KATINE, M. CAREY, L. FOLKS, O. OZATAY, B.D. TERRIS, Hitachi Global Storage Technologies, San Jose Research Center, 3403 Yerba Buena Road, San Jose CA 95135 — We study at low temperature spin transfer torque (STT) driven free-layer magnetization reversal in current perpendicular to plane (CPP) spin valves with in-plane magnetization. The precessional frequencies of the direct current driven pre-switching modes were measured. Based on this characterization we compare the pre-switching and switching behavior, when driven by direct currents only and in the presence of an additional rf current bias. We find interesting rf induced dynamics such as frequency locking as well as effects on the critical switching boundary. These effects appear for applied frequencies close to the dc-only driven pre-switching resonance frequencies. In particular, we observe a reduction in the critical current for switching when applying rf with frequencies slightly below this range. Macrospin simulations (using Slonczewski STT) reproduce well our experimental data and serve as a basis for the development of a phenomenological model that describes the observed behavior.

1Supported in part by NSF Grants DMR-05-01013 and DMR-06-45377
2Supported in part by HGF and by DFG through SPP1113

\(^1\)Research supported in part by NSF grant DMR-05-01013.
2:30PM L33.00001 Ultrafast coherent optical manipulation of a single electron spin in a quantum dot. M.H. MIKKELSEN, J. BEREZOVSKY, N.G. STOLTZ, L.A. COLDREN, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — A key ingredient for spin-based quantum information processing is the coherent rotation of a spin state on timescales much faster than the spin coherence time. By applying off-resonant, picosecond-scale optical pulses, we demonstrate the coherent rotation of a single electron spin in a GaAs quantum dot (QD) through arbitrary angles up to \( \pi \) rad. We directly observe this spin manipulation using time-resolved Kerr rotation spectroscopy at \( T = 10K \). Measurements of the spin rotation as a function of laser detuning and intensity confirm that the optical Stark effect is the operative mechanism and the results are well-predicted by a model including the electron-nuclear spin interaction. Using short tipping pulses and QDs with long spin coherence times, this technique enables one to perform a large number of operations within the coherence time.

We acknowledge support from NSF and AFOSR.


2:42PM L33.00002 Coherent Population Trapping of an Electron Spin in a Singly-Charged Quantum Dot. XIAODONG XU, BO SUN, PAUL R. BERMAN, DUNCAN G. STEEL, The Physics Department, The Univ. of Michigan, ALLAN S. BRACKER, DAN GAMMON, Naval Research Lab. LU J. SHAM, The Physics Department, The Univ. of California, San Diego — When two radiation fields drive coupled transitions in a three-level lambda system, a steady-state coherent superposition of the ground states can be formed in which the system is totally decoupled from the applied fields, a process that is sometimes referred to as coherent population trapping (CPT). Here we report the demonstration of the CPT of an electron spin in a singly-charged quantum dot. By applying a magnetic field in the Voigt geometry, we create a three-level lambda system, formed by two Zeeman sublevels of an electron spin and an intermediate trion state. As we tune the driving and probe fields to the two-photon Raman resonance, we observe a pronounced dip in the probe absorption spectrum, indicating the CPT of the electron spin. An arbitrary superposition of the electron spin states can be prepared by varying the ratio of the Rabi frequencies between the driving and probe fields. This work shows that spin based semiconductor quantum dot systems can exhibit the same interesting quantum behavior that has been found in simple atom-field systems.

This work was supported in part by U.S. ARO, AFOSR, ONR, NSA/LPS, and FOCUS-NSF.

2:54PM L33.00003 Spin polarized current generation from quantum dots without magnetic fields. JACOB J. KRICH, BERTRAND I. HALPERIN, Harvard University — An unpolarized charge current passing through a chaotic quantum dot with strong spin-orbit coupling can produce a spin polarized exit current without magnetic fields or ferromagnets. If there is only one channel in the output lead, no spin polarization can be produced. We use random matrix theory to estimate the typical spin polarization as a function of the number of channels in each lead, finding rms spin polarizations up to 45% with one input channel and two output channels. Finite temperature and dephasing both suppress the effect, and we include dephasing effects using a new variation of the third lead model.

This work has been supported in part by NSF grants PHY-06-46094 and DMR-05-41988 and the Fannie and John Hertz Foundation.

3:06PM L33.00004 The role of electron-hole exchange in the spin mixing of excited-shell excitons in quantum dots. STEFAN C. BADESCU, THOMAS L. REINECKE, U.S. Naval Research Laboratory — In semiconductor quantum dots (QDs) the long-range electron-hole exchange is known to lift the spin degeneracy of ground orbital state excitons for small lateral asymmetries. In the context of solid-state quantum computing recent developments in optical manipulation of spin involve the excited shells of charged excitons in single and coupled QDs. We demonstrate here that this electron-hole exchange is important in the mixing of spin states of excitons in higher shells in QDs, e.g., the p-shell exciton. In contrast to the ground states, no lateral asymmetry is necessary for simultaneous reversal of an electron and a hole spin in these excited shells. For charged excitons, this interaction competes with the asymmetric exchange between electrons or between holes. We discuss the optical selection rules and the role of dephasing from phonons for the dynamics of excited excitons. We conclude that the e-h exchange is an important factor in designing logical gates with excited states.

This work is supported by the Office of Naval Research.

3:18PM L33.00005 Theoretical Study of Dynamical Nuclear Spin polarization in Semiconductor Quantum Dots. CHIA-WEI HUANG, XUEDONG HU, University at Buffalo, The State University of New York — Dynamical nuclear spin polarization (DSP) can be achieved optically in a semiconductor quantum dot (QD) via the hyperfine interaction between the optical oriented electron and nuclear spins. Here we explore several mechanisms, combined with the hyperfine interaction, to investigate how efficiently they can transfer the electron spin polarization to nuclei. Specifically, to ensure energy conservation during the spin transfer, we consider both a combination of electron spin-orbit and electron-phonon interactions, and cotunneling processes. Based on these interactions we evaluate the buildup time for DSP in a semiconductor QD. Our results show that the DSP buildup time of spin-orbit associated with the hyperfine interaction, accompanied by phonon emission, is of the order of seconds. This is much longer than that of the recent experimental findings. [1] The calculated nuclear spin polarization rate also shows a different Zeeman-energy-dependence from what is observed experimentally. [1] We thus conclude that hyperfine interaction combined with electron level broadening due to cotunneling processes between the QD and the nearby reservoir is more likely to be responsible for the fast buildup of nuclear polarization in experiments. [1] We have studied the emission spectra from InAs quantum dots as a function of carrier spin polarization; experiment and theory. [1] I. KHAN, T. ALI, M. YASAR, A. PETROU, SUNY at Buffalo, G. KIOSEOGLOU, C.H. LI, A.T. HANIBICKI, B.T. JONKER, Naval Research Laboratory, Washington DC, M. KORKUSINSKI, P. HAWRYLAK, Institute for Microstructural Sciences NRC, Ottawa — We have studied the emission spectra from InAs quantum dots (QDs) under the following conditions: a) recombination of spin-polarized electrons with unpolarized holes; b) recombination of spin-polarized electrons with spin-polarized holes. In the first experiment (a), we recorded the electroluminescence from Fe/GaAs n-i-p spin-LEDs which incorporate a single layer of InAs QDs at the center of the intrinsic region of the device. In the second experiment (b), we studied the photoluminescence spectra from a similar undoped heterostructure using optical pumping. In both experiments, in addition to the typical shell structure of the emission spectra, new polarization maxima are observed on the high and low energy sides of the shell emission features as a result of the imbalance between the two spin populations of the carriers. These results are compared with a calculation for the case of two and six electron-hole occupancy of the QDs.

1 Work at SUNY was supported by ONR and NSF.
3:42PM L33.00007 Determination of spin polarization in InAs/GaAs self-assembled quantum dots, F. G. C. HERNANDEZ, T. P. MAYER ALEGRE, G. MEDEIROS-RIBEIRO, Laboratorio Nacional de Luz Sincrotron — The electronic spin in a quantum dot (QD) has been proposed as a candidate two-level system for qubit implementation in a quantum information processing scheme (QIP). For semiconductor quantum dots, the optical transition selection rules provide a natural tool for a direct and quantitative measurement of the electronic spin polarization. In contrast to the optical scheme, electrical readout of the electronic spins orientation do not require any knowledge of hole polarization. Here we perform magneto-capacitance spectroscopy measurements of QDs embedded in a Metal-Insulator-Semiconductor (MIS) capacitor structure. A statistical approach for the population of the spin levels allows one to study the spin orientation in the limit of comparable magnetic and thermal energies. The amount of polarization was inferred by measuring the addition energies of electrons sequentially loaded in QDs. In this experiment, we found an electron spin polarization higher than 50% for $B_{\text{eff}} = 4T$. Finally, by including the g-tensor anisotropy the angular dependence of spin polarization with the magnetic field $B$ orientation and strength could be explained.

3:54PM L33.00008 Non-volatile spin bistability based on ferromagnet-semiconductor quantum dot hybrid nanostructure1, YURIY SEMENOV, HANI ENAYA, North Carolina State University, JOHN ZAVADA, U.S. Army Research Office, KI WOOK KIM, North Carolina State University — Electrical manipulation of a memory cell based on bistability effect in a nanostructure consisting of a semiconductor quantum dot (QD) adjoining on opposite sides with a dielectric ferromagnetic layer (DFL) and a reservoir of itinerant holes is investigated theoretically. The operating principle is based on the interplay between the exchange field of the holes $B_h$ acting on the magnetization vector of the DFL at perpendicular to the structure plane and the anisotropy field $B_a$ which aligns $M$ along the plane. At low hole population of the QD ($B_h < B_a$), $M$ is still in plane direction (first stable state “0”). If an applied bias populates the QD sufficiently ($B_h > B_a$), the subsequent $M$ rotation will decrease the hole energy in the QD; hence the high hole population state is sustained (second stable state “1”) under a fixed electro-chemical potential set by the reservoir even after bias is removed. The analysis of bit retention time of the proposed memory demonstrates the feasibility of the device with lateral QD size at least 30 nm under room temperature operation. Another advantage is the extremely small dissipative energy for Write/Erase operations.

4:06PM L33.00009 Method for Full Bloch-Sphere Control of a Localized Spin in a Quantum Dot via a Single Electrical Gate, JOSEPH PINGENOT, CRAIG E. PRYOR, MICHAEL E. FLATTE, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa — Manipulating individual spins in solids requires quickly and coherently reorienting localized spins while leaving neighboring spins unaffected. Difficulties confining oscillating magnetic fields have motivated alternate approaches that use electric fields to change the local magnetic environment, including moving an electron within a hyperfine field gradient or fringe-field gradient. Higher temperatures require spins to be localized in much smaller quantum dots, where these techniques are less effective. In contrast, g-tensor manipulation techniques[1] couple an electric field to the spin via the spin-orbit interaction, and should be scalable to small dots with large confinement. Here we calculate the g-tensor of a single electron in a small quantum dot and show the symmetry of its electric field dependence permits full Bloch sphere control of the spin using an electric field applied in a single direction. We find the spin manipulation frequency of an InAs/GaAs QD in 1 Tesla exceeds 150 MHz. We acknowledge support of an ONR MURI and an NSF NIRT. [1] Kato et al. Nature 299, 1201 (2003)

4:18PM L33.00010 Enhancement of spin lifetime in quantum well lasers using interface fluctuation quantum dots, RYAN WOODWORTH, Pennsylvania State University, ARI MIZE, Science Applications International Corporation, RUSKO RUSKOV, Ames National Laboratory, GERALD MAHAN, Pennsylvania State University — Research on semiconductor heterostructures provides many insights into the next generation of optoelectronic devices. In particular, the gain of a microdisk laser seems to be enhanced by the presence of a long-lived optical cavity mode. Here we analyze a recent experiment using GaAs-AlGaAs microdisks with interface fluctuation quantum dots. A numerical simulation shows enhancement of spin dephasing time in the conduction band due to exchange scattering and D’yakonov-Perel coupling. Possible applications to quantum computing are discussed.

4:30PM L33.00011 Piezomagnetic quantum dots1, Ramin ABOULFATH, SUNY Buffalo; University of Texas, Dallas, A.G. PETUKHOV, South Dakota School of Mines and Technology, Rapid City, IGOR ZUTIC, SUNY Buffalo — We study the influence of deformations on magnetic ordering in quantum dots doped with magnetic impurities. The reduction of symmetry and the associated deformation from circular to elliptical quantum confinement lead to the formation of piezomagnetic quantum dotsp. The strength of elliptical deformation can be controlled by the gate voltage to change the magnitude of magnetization, at a fixed number of carriers and in the absence of applied magnetic field. We reveal a reentrant magnetic ordering with the increase of elliptical deformation and suggest that the piezomagnetic quantum dots can be used as nanoscale magnetic switches. Finally, we discuss thermodynamic stability of piezomagnetism in such quantum dots.

Supported by US ONR and NSF-ECCS CAREER.


Tuesday, March 11, 2008 2:30PM - 5:18PM —
Session L35 FIAP: Optoelectronic Devices and Applications Morial Convention Center 227

2:30PM L35.00001 High Efficiency Quantum Cascade Lasers1, MATTHEW ESCARRA, ANTHONY HOFFMAN, SCOTT HOWARD, KAILE FRANZ, AISHWARYA SRIDHAR, CLAIRE GMACHL, Princeton University — Quantum cascade (QC) lasers have proven to be of great interest as powerful and versatile mid-infrared light sources. However, improvement in the wall-plug efficiency of these sources at room temperature and under continuous wave operation is critical to their development across a broad range of sensing applications. The internal, current, voltage, and optical efficiencies all must be maximized. Several different approaches must be taken. We will focus primarily on several QC laser designs with low voltage defect. Low voltage defect quantum designs with heterogenous injector regions have shown efficiencies as high as 13.9% from a single facet in 80K, pulsed operation. Performance at high temperatures can be improved by better confinement of electrons in the upper laser level. The addition of high-reflection and anti-reflection coatings to opposing facets has greatly improved the optical efficiency. Temperature performance can also be improved through InP lateral regrowth, epitope side down mounting, and electroplated gold top contacts.

This work is supported in part by DARPA-EMIL and MIRTHE (NSF-ERC).
2:42PM L35.00002 High-speed wavelength conversion in quantum-dot and quantum-well semiconductor optical amplifiers. DAVID NIELSEN, S. L. CHUANG, University of Illinois at Urbana-Champaign, N. J. KIM, D. LEE, Chongnam National University, S. H. PYUN, W. G. JEONG, Sungkyunkwan University, C. Y. CHEN, T. S. LAY, National Sun Yat-Sen University — All-optical wavelength conversion is an important technology for advanced wavelength division multiplexed networks. The carrier localization available in quantum dots, due to the relatively slow carrier capture and escape times compared to intersubband relaxation in quantum wells, makes it possible to achieve efficient wavelength conversion through the non-linear optical process of four-wave mixing due to enhanced spectral hole burning. To examine the various carrier dynamics we experimentally investigate four-wave mixing in both quantum-dot and quantum-well optical amplifiers. Our results show superior conversion efficiency in a quantum-dot device compared to a quantum well device with identical gain at pump-probe detunings between 100 GHz and 1 THz, and a small-signal modulation bandwidth > 25 GHz. Cross-gain modulation measurements were performed as well and show a much smaller bandwidth of 1 GHz indicating that four-wave mixing is superior for high-speed signals.

2:54PM L35.00003 Magnetic field controlled sub-THz emission in Quantum Cascade Lasers. A. WADE, G. FEDOROV, D. SMIRNOV, NNMFL, S. KUMAR, Q. HU, MIT, Dept of EE and CS, B.S. WILLIAMS, Univ. of California at LA, Dept of EE — We report on the observation of strong multi-wavelength terahertz (THz) radiation in GaAs/AIGAs based Quantum Cascade Lasers (QCL). The QCL was measured in a strong magnetic field, up to 31 T, applied parallel to the growth axis. The lasing intensity exhibits oscillations due to magnetophoton resonance and Landau Level interaction resulting in a strong increase in the optical power and reduction of the current threshold. By applying the appropriate magnetic field and bias, lasing emission is obtained between 3.27 to 2.61 and 1.53 to 0.68 THz. This demonstrates that a magnetic field offers the unprecedented possibility to control the QCL emission frequency and achieve lasing action as low as 0.68 THz.

3:06PM L35.00004 Effect of Waveguide Side-Wall Roughness on Quantum Cascade Laser Performance. FATIMA TOOR, HAO LIU, Princeton University, DEBORAH SIVCO, Alcatel-Lucent, CLAIRE GMACHL, Princeton University — Waveguide loss in optical devices can be attributed to two main factors, intrinsic material loss (e.g. free carrier absorption) and scattering loss from imperfections (e.g. fabrication errors). To-date most work for determining the waveguide loss of quantum cascade lasers (QCLs) is concentrated on determining the intrinsic material loss, but there is very little research work done on determining the effect of fabrication errors such as side-wall roughness on QCL performance. Here, we report on an experimental and modeling study to determine the effect of side-wall roughness on QCL laser performance. The work involved designing and fabricating waveguides with different amounts of side-wall roughness. Measurements were then taken to determine the effect of waveguide side-wall roughness on laser performance parameters like threshold current density and slope efficiency.

3:18PM L35.00005 Optical coherence imaging using the phase coherent photorefractive effect in ZnSe quantum wells. A. KABIR, M. AJWARD, S. TRIPATHY, H.P. WAGNER, Department of Physics, University of Cincinnati, OH 45221, U.S.A. — We have performed depth-resolved optical coherence imaging (OCI) of both stationary and moving objects using the exciton resonant phase coherent photorefractive (PCP) effect in ZnSe quantum wells (QWs). PCP QWs operate without electrical contacts thus avoiding elaborate sample processing and avoiding sample destruction due to Joule heating. In addition, the PCP effect exploits the coherence of excitons in OCI experiments thus enabling 3D images of reflecting objects with a depth resolution of ∼2 µm using 90 fs pulses. Due to the high diffraction efficiency of η ∼ 10~4 in our PCP ZnSe QWs we are able to record still images at very low intensities (∼500 µW/cm~2). The OCI movies of moving objects were recorded using a camcorder with frame rates of 60 and 180 Hz. The shortest possible time resolution in these experiments is determined by the decay time of the PCP electron grating being in the 10~6 range.


3:42PM L35.00007 High precision frequency characterization of THz quantum cascade lasers by heterodyne mixing. MARK LEE, MICHAEL WANKE, MAYTEET LERTTAMRAB, ERIK YOUNG, ALBERT GRINE, JOHN RENO, Sandia National Laboratories, ROBERT DENGLER, PETER SIEGEL, Jet Propulsion Laboratory - Cal Tech — Terahertz quantum cascade lasers (QCLs) have been used together with a monolithic planar Schottky diode receiver to study the heterodyne mixing between dual internal modes of a QCL and between a single mode of a QCL and a known molecular line from a molecular gas laser. Dual mode mixing using a single QCL shows that the intrinsic linewidth of a free-running QCL is < 30 kHz. Both a grating and distributed feedback grating QCLs were mixed against known molecular gas laser lines. Resulting difference frequency spectra gave a high precision measurement of a QCL’s absolute frequency against known references. Unusual slow transient turn-on behavior was also observed in a pulsed standard QCL. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:54PM L35.00008 Electric Field and Polarization Dependent Spatial Fringe-Patterns in Electro-optic Crystals. RANDALL HINTON, ANTHONY GARZARELLA, DONG HO WU, Naval Research Laboratory/ Temple University — Electro-optic (EO) crystals, such as LiNbO3, are being widely used for high speed optical communication applications, which exploit their fast EO modulation capability. This EO modulation capability is also being used for the detection of an electric field over an extremely broad frequency band, namely DC through THz. It is known that most of EO crystals exhibit the photorefractive, pyroelectric, piezo and photo-electric effects. While considered as parasitic effects and detrimental for most EO applications, our experimental results seem to suggest that some of these effects can increase the effective EO responsivity. To understand how these effects influence the EO responsivity we have carried out systematic investigations with LiNbO3 and Sr0.75Ba0.25Nb2O6 crystals. When a linearly polarized laser beam (628 nm) passes through the crystal, to which an external low frequency AC field is applied, we observed a periodic interference pattern, which was dynamically modulated by the AC field. We also found that the interference pattern was produced by the reflected beam from the crystal’s front and back surfaces. The patterns and dynamic modulation behaviors of the transmitted and reflected beams were noticeably different from each other. We will discuss the implications of these experimental results to the EO responsivity.
4:06PM L35.00009 A MHz-Rate High-Power UV Laser Source for High-Speed Planar Laser-Induced Fluorescence Spectroscopy, MIKHAEL N. SLIPCHENKO, JOSEPH D. MILLER, TERRENCE R. MEYER, Department of Mechanical Engineering, Iowa State University, Ames IA 50011; NAIEO JIANG, WALTER R. LEMPERT, Departments of Mechanical Engineering and Chemistry, The Ohio State University, Columbus, OH 43202, JAMES R. GORD, Air Force Research Laboratory, Propulsion Directorate, Wright-Patterson AFB, OH 45433 — We report on producing MHz-rate pulse burst tunable high energy UV radiation and its application to high-speed temperature measurements of combustion based on planar laser-induced fluorescence (PLIF) spectroscopy. The laser system consists of a narrowband high-speed tunable seeded OPO pumped by harmonics of a MHz-rate pulse-burst pump laser. The pump laser utilizes an AOM-based pulse slicer followed by a 5-stage Nd:YAG amplifier. The pump laser produces 4 bursts per second with a burst duration as long as 1.5 ms and total burst power up to 2 J. Each burst consists of 5 to 100 pulses with each pulse duration variable between 6 to 50 ns. The custom OPO produces up to 5 mJ per pulse in the range from 220 to 315 nm for exciting electronic transitions of species such as nitric oxide and the hydroxyl radical. The laser system performance is tested in well characterized flames and pulse-burst PLIF results are presented.

4:18PM L35.00010 Theory of THz rectification at a gate controlled Shottky barrier in a FET based plasmonic detector, G.R. AIizin, J. MIKALOPAS, CUNY, New York, G.C. DYER, UC Santa Barbara, E.A. SHANER, M.C. WANKE, Sandia National Laboratories, S.J. ALLEN, UC Santa Barbara — We present a theory of the resonant THz photoresponse in a grating gated FET with a gate controlled Shottky barrier [1]. We use theoretical modeling to show that the potential barrier induced in the 2D FET channel by an isolated gate finger, biased to pinch off, yields the Shottky-like I – V characteristics of the FET. The gate coupling causes an external THz radiation to the plasmon excitations in the 2D electron channel. We calculate the photoresponse signal resulting from the THz rectification at the Schottky barrier and demonstrate that it has resonant peaks at plasmon frequencies. The results obtained are consistent with recent measurements [2]. This work is supported by ARO (Grant # W911NF-05-1-0031) and The University at Buffalo NSF NIRT (Grant # ECS0609146 ). Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. 1. E.A. Shaner et al, Appl. Phys. Lett., 90, 181127 (2007). 2. G. Dyer et al, this meeting presentation.

4:30PM L35.00011 Control of exciton fluxes, ALEX HIGH, AARON HAMMACK, E.E. NOVITSKAYA, LEONID BUTOV, University of California at San Diego, MICAH HANSON, ARTHUR GOSSARD, University of California at Santa Barbara — We present proof of principle for control of excitonic fluxes by gate in mesoscopic devices. Since excitons are bosonic particles, control of exciton fluxes can extend mesoscopics, the field which electron transport in transport provides. Also, as are coupled to light, the control of exciton fluxes may lead to development of new optoelectronic devices. The demonstrated devices as a directional switch, star switch, and flux merger.

4:42PM L35.00012 Experimental Studies of Alignment Tolerance and High Temperature Performance of A Fabry-Perot Interferometric Pressure Sensor, IVAN PADRON, ANTHONY FIORY, NUGGEHALLI RAVIDNRA, New Jersey Institute of Technology — Fabry-Perot interferometry is one of the most reliable of the several optical techniques that can be utilized to facilitate the fabrication of an optical sensor. Devices based on this technique can provide high degree of sensitivity, versatility and immunity to environmental noise. The Fabry-Perot Interferometric Sensor (FPIS), to be discussed in this presentation, consists of a Fabry-Perot cavity formed between two bonded surfaces: a corrugated diaphragm with a center rigid body (or boss) which deflects under internal pressure and keeps a high alignment tolerance and a glass surface with an optical fiber insert. The Fabry-Perot cavity and optical fiber have been used as the sensing element and interconnect, respectively. The Fabry-Perot cavity has been fabricated using the MEMS technology. Micromachining techniques make Fabry-Perot sensors very attractive by reducing the size and cost of the sensing element.

4:54PM L35.00013 Growth and properties of wide band gap II-VI multi-quantum well structures for mid-infrared quantum cascade lasers, WILLIAM CHARLES, The City College of New York, KALE FRANZ, Princeton University, AIDONG SHEN, MARIA TAMARGO, The City College of New York, CLAIRE GMACHL, Princeton University — Mid-infrared emission based on intersubband transitions has been recently very actively pursued for the fabrication of quantum cascade lasers (QCLs) operating in that wavelength range. Highly efficient, ultra fast lasing can be achieved from engineered structures in which the emission wavelength is determined by the precisely controlled multi-layered structure rather than the specific materials of choice. However, operation at wavelengths shorter than 3.5 μm is limited by the conduction band offset of the materials currently available. To address this limitation, we have begun to explore wide band gap II-VI ZnCdMgSe materials grown lattice matched to InP substrates for these applications. Recently, we reported the growth and characterization of multi-quantum well structures that exhibit absorption in the 3-5 μm region. We have designed a structure consisting of the active/injector regions of a QCL and fabricated electroluminescent devices. Electroluminescence emission at 4.7 μm has been observed in these structures, suggesting that these materials hold great promise for the fabrication of short wavelength mid-IR QCLs. This work is supported by NSF Grant No. EEC-0540832 (MIRTHE-ERC).

5:06PM L35.00014 Behavior of laser diodes in the small particle number quantum limit, KAUSHIK ROY CHAUDHURY, ANTHONY F.J. LEVI — We use master equations to model the steady-state and transient response of a laser diode in the small particle number quantum limit. In scaled laser diodes n electrons and s photons are correlated such that <ns> may not be factorized and there are significant differences in behavior compared to predictions of continuum mean-field theory. Quantization of photon number is found to suppress lasing threshold and create a non-Poisson probability distribution for n discrete electrons and s discrete photons. The same correlation effect dampens the transient dynamic response of laser emission. The predictions of conventional mean-field and Langevin theory are recovered in the large particle number limit.
Understanding Atomistic Mechanisms for Reversible Hydrogen Storage in Metal Hydrides: Application to Alane Formation on Ti Doped Al Surfaces

We describe a density functional kinetic Monte Carlo approach enabling us to study and simulate the steady-state situation of dissociative adsorption of hydrogen along with diffusion and reaction of Al and H atoms leading towards the formation of alane species on Ti-doped Al surfaces. In the first step, density functional theory is used in conjunction with the nudged elastic band/drag method to obtain the energetics of the relevant atomistic processes of Al and H diffusion and their reactions on Al surfaces with different concentration of dopant Ti atoms. Subsequently, the kinetic Monte Carlo method is employed, which accounts for the spatial distribution, fluctuations, and evolution of chemical species at Ti-doped Al surfaces under steady-state conditions. This DFT-based KMC approach provides an insight into the kinetics of alanes at technologically relevant pressure and temperature conditions. Our computed production rates of AlH3 on Al surfaces are in agreement with experimental data. We also obtained temperature programmed desorption spectra of different alane species, which is agreeing well with experiments.

3:06PM L36.00002 Density Functional Theory Based Kinetic Monte Carlo Approach for Understanding Atomistic Mechanisms for Reversible Hydrogen Storage in Metal Hydrides: Application to Alane Formation on Ti Doped Al Surfaces1, A. KARIM, J. MUCKERMAN, P. SUTTER, E. MULLER, BNL — We describe a density functional kinetic Monte Carlo approach enabling us to study and simulate the steady-state situation of dissociative adsorption of hydrogen along with diffusion and reaction of Al and H atoms leading towards the formation of alane species on Ti-doped Al surfaces. In the first step, density functional theory is used in conjunction with the nudged elastic band/drag method to obtain the energetics of the relevant atomistic processes of Al and H diffusion and their reactions on Al surfaces with different concentration of dopant Ti atoms. Subsequently, the kinetic Monte Carlo method is employed, which accounts for the spatial distribution, fluctuations, and evolution of chemical species at Ti-doped Al surfaces under steady-state conditions. This DFT-based KMC approach provides an insight into the kinetics of alanes at technologically relevant pressure and temperature conditions. Our computed production rates of AlH3 on Al surfaces are in agreement with experimental data. We also obtained temperature programmed desorption spectra of different alane species, which is agreeing well with experiments.

1Work performed in collaboration with Amra Peles, and supported by the Department of Energy and by the University of California Energy Institute.

3:18PM L36.00003 Alanes formation on the Al(111) surface, SYLVIE RANGAN, JEAN-FRANCOIS VEYAN, YVES J. CHABAL, University of Texas at Dallas, SANTANU CHAUDHURI, Washington State University, JAMES T. MUCKERMAN, Brookhaven National Laboratory — Alane clusters (AlH3) are believed to be the ubiquitous intermediates in hydrogen storage reactions for a wide variety of alanates (LiAlH4, NaAlH4) currently considered for hydrogen storage. The formation and behavior of alanates at surfaces appear to control and limit the efficiency of hydrogen storage. In particular, hydrogen adsorption on the Al(111) surface leads to the coexistence of several adsorbed species, the concentration of which is affected by the step density, the surface coverage and the temperature. We combine density functional theory (DFT) and surface infra-red (IR) absorption spectroscopy to uncover the mechanisms for alane formation on Al(111) surfaces. At low coverage, DFT predicts a two-fold bridge site adsorption for atomic hydrogen, consistent with previous Electron Energy Loss Spectroscopy measurements. At higher coverage, the formation of small chemisorbed AlH3 occurs at the step edges. With increasing coverage AlH3 is extracted from the step edge and becomes highly mobile on the terraces in a weakly bound state. This mobility is the key factor leading to the growth of larger alanates through AlH3 oligomerization. For these large alanates, previous Thermal Programmed Desorption studies are discussed and compared to the thermal stability observed in IR.

3:30PM L36.00004 Watching the dehydrogenation of alane (AlH3) in a TEM, SHANE BEATTIE, TERRY HUMPHRIES, LOUISE WEAVER, SEAN MCGRADY, University of New Brunswick — Alane (AlH3) is a promising candidate for on-board hydrogen storage applications. Its theoretical gravimetric capacity is 10.1 percent and decomposition is achieved with modest heating (60-200 deg C). We studied the dehydrogenation of alane, insitu, in a TEM. Alane powder was loaded into the TEM and heated at 80 deg C. We were able to watch the dehydrogenation of the alane to aluminum. Electron diffraction and dark field images are used to show how and where the aluminum crystallites grow. Although crystalline aluminum phases were successfully identified, some of the sample remained amorphous. We will discuss the nature of the amorphous material and present images clearly identifying the nature of the aluminum crystallites.

3:42PM L36.00005 Hydrogen Multicenter Bonds on Small Metal Clusters1, P. TARAKESHWAR, T.J. DHILIP KUMAR, N. BALAKRISHNAN, Department of Chemistry, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89114, USA — We investigate the saturation of hydrogen on metal clusters employing ab initio calculations. Our calculations reveal that energetically the most preferred configuration of the hydrogen saturated metal clusters exhibit hydrogen multicenter bonds. The strength of these hydrogen multicenter bonds can be modulated either by changing the extent of hydrogen saturation or using different metal clusters. In the context of hydrogen storage materials, our calculations indicate that early first-row transition metals have the best propensity to form hydrogen multicenter bonds. The relevance of this work in the context of hydrogenation and dehydrogenation kinetics of complex metal hydrides will be discussed.

1This work is supported by DOE Grant DE-FG36-05GO85028.

3:54PM L36.00006 The absorption of hydrogen by Nb thin films capped with Pd studied by transmission of visible light1, J. I. AVILA, A. L. CABRERA, Facultad de Fisica, Pontificia Universidad Catolica de Chile, G. B. CABRERA, DAVID LEDERMAN, Department of Physics, West Virginia University, Morgantown — Samples of Nb films with thickness between 2.5 to 14 nm were deposited on glass and capped by a continuous 6 nm Pd film in a sputtering system. The light transmission and reflection, in the visible range (400 to 1000 nm), were measured when the sample was exposed to different hydrogen pressure up to 75 Torr. Experiment on continuous pure Pd film and Nb film were done for comparison. The relative change in transmission for Nb at 74 Torr of hydrogen is about 5 percent but the saturation occurs after 2500 s. A sample of 14 nm Nb capped by Pd showed a 2 percent increase in transmission at the same pressure but the saturation time is reduced to 50 s, same as pure Pd. Change in the kinetics of hydrogen absorption by Nb capped with Pd indicates that the rate limiting step in the absorption process by pure Nb is located on the Nb surface.

1Funding by FONDECYT grant #1060634/Chile and NSF CIAM grant DMR-0502825.
4:06PM L36.00007 Theoretical Analysis on X-ray Absorption Spectra of Ti compounds as Catalysts in Lithium Amide-Imide reactions, TAKAO TSUMUYARA, TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Solid-state storage is conceptually efficient approach for on-board vehicular hydrogen storage. In this context, light-element materials such as lithium amide LiNH$_2$ and lithium imide Li$_2$NH have been attracted much attention due to their high gravimetric densities of hydrogen. Recently, various transition-metal compounds have been examined with ball-milling technique for exploring catalysts to improve the hydrogen storage and desorption kinetics, and it is found that a small amount (1mol%) of titanium compounds revealed a superior effect in hydrogen desorption reaction LiNH$_2$ + LiH $\rightarrow$ Li$_2$NH + H$_2$ [1]. However, these catalysts mechanism and role of Ti in the reaction remain unanswered. Isobe et al. have carried out measurements of X-ray absorption spectroscopy(XAS) at Ti K-edge to see the electronic states of Ti recently [2]. In this paper, we calculate the electronic structure of Ti metal and its compounds, and obtained theoretical spectra to compare with the measured spectra by using first-principles calculations based on the all-electron FLAPW method. We discuss chemical bonding and local geometry of catalytically active states in the reaction. [1] T. Ichikawa, S. Isobe, N. Hanada and H. Fujii, J. of Alloys and Comp. 365, 271 (2004). [2] S. Isobe, T. Ichikawa, Y. Kojima and H. Fujii, J. of Alloys and Comp. 446-447, 360 (2007).

Tuesday, March 11, 2008 2:30PM - 5:18PM — Session L37 DCMP: Semiconductors II: Structure and Phase Diagrams Morial Convention Center 229

2:30PM L37.00001 First-Principles epitaxial phase-diagram, short-range order, microstructure and electronic properties of (In,Ga)N zincblende alloys on GaN$^1$, ZHE LIU, PAULO PIQUINI, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — A first-principle total energy cluster expansion method is developed to study thermodynamic properties of epitaxial semiconductor alloys coherent to substrate (i.e., $<critical$ $thickness$ $h_c$), in which coherent strain energy as a function of atomic configuration is explicitly described. The search for epitaxial ground state structures of (In,Ga)N alloy grown on GaN (001) substrate concludes that epitaxial strain suppresses phase separation, which is normally observed for bulk (In,Ga)N alloy and relaxed films. Two (102) superlattices: (InN)$_2$/(GaN)$_2$ and (InN)$_3$/(GaN)$_3$, are determined to be the epitaxial ground state structures. Composition-temperature phase diagram calculated by Monte Carlo method shows that homogeneous solid solution phase is thermodynamically stable at typical growth temperature of blue and green LED by MBE and MOCD (x/ln~0.20~0.30 and $h_c$ ~10~30nm). Such calculated phase diagram can be used to understand the controversy regarding atomic microstructures in (In,Ga)N quantum well devices. Short-range-ordering of the solid solution phase and its influence on the electronic properties are also discussed.

$^1$Funded by DOE-SC-BES-DMX

2:42PM L37.00002 First principles and valence force field study of III-V quaternary alloys$^1$, KOUSHIK BISWAS, ALBERTO FRANCESCHETTI, STEPHAN LANY, National Renewable Energy Laboratory — We report on the elastic properties and formation energies of Ga$_x$In$_{1-x}$P$_y$N$_{1-y}$-quaternary alloys using first principles and valence force field (VFF) calculations. The elastic constants of the binary compounds (GaP, InP, GaN, and InN) were calculated using the local density approximation (LDA). The resulting VFF parameters, $\alpha$ (bond stretching) and $\beta$ (bond angle bending) were used within the Keating model to calculate the formation energies of GaNP, GaN, InP, and GaPN ordered structures. We found that the VFF formation energies of phosphide-nitride alloys (e.g. GaPN) were not in very good agreement with the LDA formation energies. Conventionally, the bond bending parameter $\beta$ for a ternary alloy is chosen as the arithmetic mean of the binary constituents. To improve the accuracy of the VFF model, we lifted such restriction on the $\beta$-parameter and we also introduced the parameter $\sigma$ (bond length-bond angle interaction). The VFF parameters $\alpha$, $\beta$, and $\sigma$ were fitted to the LDA-calculated formation energies of a large number of ternary ordered structures and were used to calculate the formation energy of the Ga$_x$In$_{1-x}$P$_y$N$_{1-y}$-quaternary alloy.

$^1$This work was funded by the U.S. Department of Energy under Contract No. DE-AC36-99GO10337 to NREL, and within NREL’s Laboratory Directed Research and Development Program.

2:54PM L37.00003 First Principles Phase Diagram Calculation For Al$_x$Ga$_{1-x}$N, JEREMY NICKLAS, JOHN WILKINS, Ohio State University — First principles phase diagram calculations were performed for the wurtzite and zincblende structures of the quasibinary system AI$_2$Ga-N. The cluster expansion method using the code ATAT was performed without and with excess vibrational contributions to the free energy, $F_{vib}$. The ab initio calculations were performed with VASP using the PAW pseudopotentials with PBE for the exchange and correlation energies. Preliminary results show miscibility gaps for both structures with a decrease in the consolute points, $(X_C, T_C)$, when including $F_{vib}$. The wurtzite structure is predicted to be approximately symmetric while the zincblende is predicted to be quite assymmetric.

3:06PM L37.00004 Simulation studies of GST phase change alloys, GLENN MARTYNA, IBM Research — In order to help drive post-Moore’s Law technology development, switching processes involving novel materials, in particular, GeSbTe (GST) alloys are being investigated for use in memory and eFuse applications. An anneal/quench thermal process crystallizes/amororphizes a GST alloy which then has a low/high resistance and thereby forms a readable/writeable bit; for example, a “one” might be the low resistance, conducting crystalline state and a “zero” might be the high resistance, glassy state. There are many open questions about the precise nature of the structural transitions and the coupling to electronic structure changes. Computational and experimental studies of the effect of pressure on the GST materials were initiated in order to probe the physics behind the thermal switching process. A new pathway to reversible phase change involving pressure-induced structural metal insulator transitions was discovered. In a binary GS system, a room-temperature, direct, pressure-induced transformation from the high resistance amorphous phase to the low resistance crystalline phase was observed experimentally while the reverse process under tensile load was demonstrated via ab initio MD simulations performed on IBM’s Blue Gene/L enabled by massively parallel software. Pressure induced transformations of the ternary material GST-225 (Ge$_2$Sb$_2$Te$_5$) were, also, examined In the talk, the behavior of the two systems will be compared and insight into the nature of the phase change given.

3:18PM L37.00005 Local structure and Phase transition of (GeTe)$_n$(Sb$_2$Te$_3$)$_m$ pseudo-binary system for the phase-change memory, JINO IM, JAE-HYEON EOM, JISUON IHM, Department of Physics and Astronomy, Seoul National University, Seoul, Korea — A theoretical investigation on the local structure and phase transition between the crystalline and the amorphous phase of (GeTe)$_n$(Sb$_2$Te$_3$)$_m$ pseudo-binary system(GST) for the phase-change memory is presented. Based on the study of the coordination number for the amorphous phase of GST, the local structure of the amorphous phase of the GST is shown to be composed of the stibnite-like building block for the Sb$_2$Te$_3$ and chain-like building block for the GeTe. The phase transition between the crystalline and the amorphous phase of GST is explained by relative repositioning of these building blocks. Density functional total energy minimization calculations show that the crystallization energy and the volume change in transition also agree with experimental data.
3:30PM L37.00006 Raman scattering studies of Ge-Sb-Te nanoparticles\(^1\). CHRISTINE KIM, HAE-YOUNG SHIN, AH REUM JEONG, WILLIAM JO, SEOKHYUN YOON, Department of Physics and Division of Nano Sciences, Ewha Womans University, Seoul 120-750, Korea — We have measured Raman scattering spectra of Ge-Sb-Te (GST) nanoparticles which are synthesized by a pulsed laser ablation method. The nanoparticles were grown under different growth conditions such as temperatures and/or pressures. Our measurements could provide information towards the optimal growth conditions for better crystalline quality of the GST nanoparticles. We have also measured nitrogen-doped GST nanoparticles. Comparison between Raman responses of nitrogen- doped- and undoped-GST nanoparticles will be presented. Our results suggest that Raman scattering spectroscopy can be used to study phases and phase changes through local structural information in the GST nanoparticles, which are being developed for low-power non-volatile memory applications.

\(^1\)Supported by the Korea Research Foundation Grant funded by the Korean Government. (KRF-2006-005-J04001)

3:42PM L37.00007 Theory of unsaturated silicon lattices\(^1\), FENG ZHANG, DAVID STUCKE, DRAGAN STOJKOVIC, VINCENT CRESPI — Several molecules are known to contain stable silicon double or triple bonds that are sterically protected by bulky side groups. Through first-principles computation, we demonstrate that well-defined \(\pi\) bonds can also be formed in two prototypical crystalline Si structures: Schwarzite Si-168 and dilated diamond. The sp\(^2\)-bonded Si-168 is thermodynamically preferred over diamond silicon at a modest negative pressure of -2.5 GPa. Ab-initio molecular dynamics simulations of Si-168 at 1000 K reveal significant thermal stability. Si-168 is metallic in density functional theory, but with distinct \(\pi\)-like and \(\pi^*\)-like valence and conduction band complexes just above and below the Fermi energy. A bandgap buried in the valence band but close to the Fermi level can be accessed via hole doping in semiconducting Si\(_{14}\)B\(_2\). A less-stable crystalline system with a silicon-silicon triple bond is also examined: a rare-gas intercalated open framework on a doped diamond lattice.

\(^1\)Supported by the National Science Foundation (CMS-0510057 and CMMI-0645953) and the National Center for Supercomputing Applications (TG-DMR08005N).

3:54PM L37.00008 Phase diagram of silicon using a DFT-based neural network potential. OLIVIERO ANDREUSSI, Scuola Normale Superiore di Pisa, Italy & DMSE, Massachusetts Institute of Technology, USA. JOERG BEHLER, Ruhr-Universitaet Bochum, Germany, MICHELE PARRINELLO, ETH Zurich, Switzerland — The phase diagram of silicon is computed by means of Classical Molecular Dynamics. A variety of Ge nanostructures formed on intact Si(111) have been observed. However, the fine structures of the atomic arrangements in the Ge nanostructures have remained elusive. We performed scanning tunneling microscopy observations and first-principle calculations for investigating the fine structures of the Ge nanostructures on the Si(111)-7\times7 surface. We obtained atomic structures of the nanostructures formed with a certain process involving deposition at temperature of 423 K and annealing at 550 K. We found that Ge nanocluster, located predominately in the faulted half unit cells of the Si(111)-7\times7 surface, contained approximately six Ge atoms with three bonded center Si adatoms. We also observed that the obtained nanostructures were stable up to 600 K.

3:46PM L37.00009 Fine Structures of Ge Nanoclusters on Si(111): STM Observations and First-Principles Theory\(^1\), A.S. RAO, University of Tulsa, H.F. MA, M.C. XU, D.X. SHI, H.J. GAO, Chinese Academy of Sciences, R. GUDIPATI, H.L. DANG, SANJU WANG, University of Tulsa — Germanium-based nanoclusters grown on silicon substrates have potential applications in optoelectronics and nanotechnology. A variety of Ge nanostructures formed on intact Si(111) have been observed. However, the fine structures of the atomic arrangements in the Ge nanostructures have remained elusive. We performed scanning tunneling microscopy observations and first-principle calculations for investigating the fine structures of the Ge nanoclusters on the Si(111)-7\times7 surface. We obtained atomic structures of the nanostructures formed with a certain process involving deposition at temperature of 423 K and annealing at 550 K. We found that Ge nanocluster, located predominantly in the faulted half unit cells of the Si(111)-7\times7 surface, contained approximately six Ge atoms with three bonded center Si adatoms. We also observed that the obtained nanostructures were stable up to 600 K.

\(^1\)Supported by the National Science Foundation (CMS-0510057 and CMMI-0645953) and the National Center for Supercomputing Applications (TG-DMR08005N).

4:06PM L37.00010 Damping of high amplitude phonons in bismuth: classical and quantum mechanical simulations. EAMONN MURRAY, Rutgers University, AARON HURLEY, University College Cork, Ireland, DAVID PRENDERGAST, Lawrence Berkeley Laboratory, TADASHI OGITSU, Lawrence Livermore National Laboratory, DAVID FRITZ, Stanford Linear Accelerator Center, DAVID REIS, University of Michigan, STEPHEN FAHY, University College Cork, Ireland — Using both classical and quantum mechanical simulations together with first-principles results, we investigate the damping mechanism of high amplitude excitations in the \(A\text{g}\) phonon mode in bismuth. Pump-probe experiments using ultrafast lasers can generate and measure large amplitude coherent oscillations of the \(A\text{g}\) phonon mode in bismuth. A substantial reduction in the lifetime of the phonon is observed when higher amplitude oscillations are produced. With third-order couplings obtained from first-principles calculations we calculate the rate of energy loss from the \(A\text{g}\) mode over several picoseconds. We find that as the highly excited \(A\text{g}\) mode decays, it produces highly excited modes in relatively small regions of the Brillouin Zone, leading to an increase in the decay rate into these modes. We show how this can greatly affect the observed lifetime of the high amplitude excitation of the \(A\text{g}\) mode.

4:30PM L37.00011 Structure of Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{6+\delta}\) supermodulation from ab initio calculations\(^1\). Y. HE, Quantum Theory Project, U. Florida, S. GRASER, P.J. HIRSCHFELD, H.-P. CHENG, Physics Dept., U. Florida — We present results of density functional theory (DFT) calculation of the structural supermodulation in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{6+\delta}\), structure, and show that the supermodulation is indeed a spontaneous symmetry breaking of the nominal crystal symmetry, rather than a phenomenon driven by interstitial O dopants. The structure obtained is in excellent quantitative agreement with recent x-ray studies, and reproduces several qualitative aspects of scanning tunnelling microscopy (STM) experiments as well. The primary structural modulation affecting the CuO\(_2\) plane is found to be a buckling wave of tilted CuO\(_2\) half-octahedra, with maximum tilt angle near the phase of the supermodulation where recent STM experiments have discovered an enhancement of the superconducting gap. We argue that the tilting of the half-octahedra and concommitant planar buckling are directly modulating the superconducting pair interaction.

\(^1\)Supported by DOE DE-FG02-97ER45660 and DE-FG02-05ER46236.

4:42PM L37.00012 Discovery of Dynamics of Jahn-Teller Effect. DAN LIU — Taking \(S=1/2\) NaSi\(_7\)O\(_{26}\), as example, we discovered the dynamics of the Jahn-Teller effect of solids by extending the molecular frontier orbital theory from chemistry to solid state physics. At the orbital and spin levels, the dynamics of the Jahn-Teller effect is exposed to spin flipping and spontaneous orbital transition that is driven by the spin-orbital coupling to keep the angle momentum reservation. The orbital transition leads to a dramatic structural change, i.e., the JT distortion. In analogue to the single-triplet intersystem crossing of photochemistry, the JT effect is a non-adiabatic process, associated with the first-order phase transition. The JT effect agrees well with the low-dimensional, \(S=1\) Haldane gap on the basis of the antimagrine Heisenberg model, if emphasizing that the \(S=1\) parameter of Haldane gap indicates the parallel spins of neighboring orbitals, rather than the on-site parallel spins. We provide insight to understanding of the unusual structural, magnetic properties of \(S=1/2\) NaTi\(_3\)S\(_6\), as well as the \(S=1\)LiV\(_2\)O\(_4\) and \(S=3/2\) LiCrGe\(_2\)O\(_6\).
4:54PM L37.00013 Dynamics of A-B transition of the DNA double helices, HOA WANG, THOMAS CHEATHAM, PETER GANNETT, JAMES LEWIS, Department of Physics, West Virginia University, Morgantown, WV 26506 — The conformational transitions of DNA and the sensitivity of DNA structure to the surrounding environment are very relevant to its chemical and biological function and potential applications in nano-technology. Different conformations of DNA, even with the same sequence, exhibit different electronic structures, resulting in different conduction properties. We present theoretical work on the dynamical features of electronic states in the A-B transition of a model DNA duplex of \( d(C\overline{G}GCGCGG)_{2} \) (10 base-pairs, 628 atoms) as the molecule undergoes conformational changes and thermal fluctuations at room temperature. We couple state-of-the-art empirical force field molecular dynamics (MD) simulations with an \textit{ab-initio} electronic structure method based on density-functional theory, called FIREBALL. For the A-B transition, we calculated the effects of conformational change on the electronic structure for each snapshot obtained from nanosecond MD simulations.

5:06PM L37.00014 Mechanism of GeSbTe phase change materials: an \textit{ab initio} molecular dynamics study\(^1\), JEAN-YVES RATY, CÉLINE OTJACQUES, JEAN-PIERRE GASPARD, University of Liège, Belgium, CHRISTOPHE BICHARA, CRMCN, University Aix-Marseille, France — Among phase change materials, Ge2Sb2Te5 (225) is one of the most successfully used in applications. Accepted models are based on EXAFS spectra and simulate a complete reorganization of bonds during amorphization, with Ge changing from sixfold to tetrahedral coordination. We perform \textit{ab initio} MD simulations of the (225), (124) and (415) liquid alloys. We show that the crystalline, liquid and amorphous structure of these systems are similar, with very little sp3 hybridization around Ge atoms and a majority of p-sigma bonds. Using a set of quenched liquid configurations we reproduce the EXAFS measurements on the (225) composition and explain how the static Debye Waller factor due to the vacancies in the crystal phase leads to a cancellation of individual neighbors contribution to the EXAFS signal while in the amorphous, a larger coherence occurs, enhancing the EXAFS signal. The computed electrical conductivities of the three phases (cubic solid, liquid and amorphous) prove to be very different, accordingly with the experiment.

\(^1\)We acknowledge support from the FNRS, the FAME NoE, and the Clusters and Wires IAP project.

Tuesday, March 11, 2008 2:30PM - 5:30PM —
Session L39 GSNP DMP: Focus Session: Deformation and Fracture Morial Convention Center 231

2:30PM L39.00001 Strain localization as a mechanism for dynamic weakening in amorphous solids, M. LISA MANNING, JAMES S. LANCER, JEAN M. CARLSON, University of California Santa Barbara — Solids such as foams, colloids, amorphous metals and granular fault gouge are composed of particles in closely-packed, non-crystalline configurations, and small-scale mechanisms for deformation in these materials are less well-understood than those in liquids or crystals. I will discuss a mesoscopic model for these disordered solids, the theory of Shear Transformation Zones (STZs), and show that it captures macroscopic features seen in experiments as well as interesting internal dynamics such as shear banding. An important component of this model is the effective temperature, which describes the statistical distributions of particle configurations and governs plastic deformation. Shear banding occurs due to a "frozen"-time instability in the effective temperature field, and one can determine a condition for shear banding based on the initial conditions alone. I will discuss how the STZ formulation can be used as a continuum model for fault gouge and includes a mechanism by which the system can dynamically weaken.

2:42PM L39.00002 What is the structure of a polymer glass after plastic deformation?, HELENE MONTES, FRANCOIS LEQUEUX, ESPCI, PPMD, CHRISTIANE ALBA-SIMIONESCO, LCP, Orsay, FREDERIQUE CASARAS, UMR 5254, Pau, PPMD, ESPCI TEAM, LCP, ORSAY TEAM — We aim to study the effect of plastic deformation on the structure of a glassy polymer. Using neutrons scattering on a large range of length scales, and comparing samples deformed below and above \( T_g \), we show that: 1) The deformation is extremely homogeneous (or affine) for length scales above the entanglement distance 2) The crossover length scale between affine and non affine deformation is about half the one of the entanglements, and is independent of temperature below the glass transition 3) The arrangement of the polymer chain is distorted by plastic deformation at the atomic scale. We then discuss these results and compare them to the results of the simulation of Hoy and Robbins (J. Polym. Sci., 44 (2006), 3487). As a conclusion we see that the entanglements are responsible for the very homogeneous deformations, forcing the individual plastic events to propagate in the sample following the tension of the chains. Thus we conclude that the physics of the plastic deformation of polymer glasses are very different from the one of other glasses.

2:54PM L39.00003 Depinning transition in failure of disordered brittle materials\(^1\), LAURENT PONSON, California Institute of Technology, FEDERAL UNIVERSITY OF RIO DE JANEIRO COLLABORATION — Crack propagation is the fundamental process leading to material failure. However, its dynamics is far from being fully understood. In this work, we investigate both experimentally and theoretically the growth velocity \( v \) of a crack propagating in brittle materials in the limit of low velocities compared to the sound speed. The variations of \( v \) with respect to the external loading \( K_I \) are carefully measured on two kinds of brittle rocks over various orders of magnitude. The crack dynamics is shown to display two regimes, well described by a sub-critical creep law \( v \sim e^{-(K_I-K_{0})^\mu} \) with \( \mu \geq 1 \) for \( K_I < K_c \), at low velocities, and a critical behavior where \( v \sim (K_I-K_c)^\theta \), with \( \theta \approx 0.8 \) when \( K_I > K_c \). We show that these variations, as well as the value of the exponents \( \mu \) and \( \theta \), can be explained extending the theoretical framework of Linear Elastic Fracture Mechanics to inhomogeneous media. In particular, these two regimes are shown to be reminiscent of the dynamical critical transition underlying the failure of disordered brittle materials.

\(^1\)The author would like to thank Dr. Guilherme Cordeiro and Ashutosh Bindal for their help in the experiments. Financial support from the French Ministry of Foreign Affairs through the Lavoisier Program is acknowledged.

3:06PM L39.00004 Role of microstructural heterogeneities on rupture of polycrystalline materials, PHILLIP DUXBURY, Michigan State University — Grain boundary networks are the dominant heterogeneity in many polycrystalline materials, and their performance may be dramatically improved by increasing the fraction of boundaries which have either low grain boundary energy or which are special boundaries, such as coincident site lattice boundaries. Significant improvement in properties such as corrosion resistance, critical current in superconductors and mechanical strength and toughness occur, provided special percolating grain or grain boundary structures can be engineered. Nevertheless, grain boundary network correlations constrain the extent to which property improvements can be achieved. A common deleterious effect is that degraded boundaries have a tendency to cluster in linear chains leading to unexpected reductions in performance. After an introduction to the area, scaling laws and the results of large scale simulations of percolation, critical manifolds and rupture in polycrystals will be presented. In particular, deleterious effects due to grain boundary correlations will be elucidated and strategies for their mitigation will be discussed.
3:42PM L39.00005 Phase field modeling of liquid metal embrittlement$^{1}$, ROBERT SPATSCHEK, NAN WANG, ALAIN KARMA, Physics Dept. and CIRCS, Northeastern University — Liquid metal embrittlement (LME) is a phenomenon whereby a liquid metal in contact with another, higher-melting-point polycrystalline metal, rapidly penetrates from the surface along grain boundaries. This phenomenon is known to be greatly accelerated by the application of tensile stress, resulting in the rapid propagation of intergranular cracks in normally ductile materials. Although this phenomenon has been known for a long time, it still lacks a convincing physical explanation. In particular, the relationship of LME to conventional fracture mechanics remains unclear. We investigate LME using a phenomenological three-order-parameter phase field model that describes both the short scale physics of crystal decohesion and macroscopic linear elasticity. The model reproduces expected macroscopic properties for well separated crack surfaces and additionally introduces short scale modifications for liquid layer thicknesses in the nanometric range, which depend on the interfacial and grain boundary energy as well as elastic effects. The results shed light on the relative importance of capillary phenomena and stress in the kinetics of LME.

$^{1}$This research was supported by DOE grant DE-FG02-07ER16400 and the DOE Computational Materials Science Network.

3:54PM L39.00006 Atomic simulation studies of plastic deformation and dislocation patterning as a function of temperature$^{1}$, N. SCOTT WEINGARTEN, Physics Dept., Catholic Univ., ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ. — The mechanical properties of crystalline solids depend sensitively on the mechanisms controlling dislocation nucleation, motion, and patterning. To explore the role of thermal activation in these processes, we carry out atomistic Monte Carlo simulation studies of plastic deformation of 2-d single crystals at a range of temperatures. We find that at intermediate temperatures, dislocations readily coalesce to form tilt boundaries, while at high temperature, the defects remain disordered in a gas-like phase, suggesting the possibility of an order-disorder phase transition. Conversely, near $T = 0$, dislocation mobility is too low to produce patterning on short time scales, again producing disordered structures. We study also the response of a polycrystalline solid under pure compression and look at the resulting distribution of stresses. We find that the defect-rich grain boundary regions bear higher stresses than those in the bulk, in agreement with Mughrabi’s two-component composite theory. Results are compared with recent experiments by L. E. Levine et al.

$^{1}$Supported by NSF DMR-0116090, DMR-0605889, and NIST-CTCMS.

4:06PM L39.00007 Novel plastic processes in nanoindented stepped Au surfaces, VIOLETA NAVARRO, OSCAR RODRIGUEZ DE LA FUENTE, ARANTAZU MASCARAUDE, JUAN MANUEL ROJO, Univ. Complutense of Madrid, 28040 — While much work has been done recently on defect nucleation during plastic processes, mechanical properties of real surfaces have been seldom studied atomistically. Defect nucleation is well known to be critical in the mechanical behaviour of materials$^{[1]}$. But the role that surface defects play on the earliest stages of plasticity still needs to be elucidated. We approach realistic surfaces by using vicinal surfaces with a high step density. Nanoindentation with AFM and atomistic simulations have been performed on the Au(788) surface$^{[2]}$. Force vs penetration curves show a hertzian initial stage and a later incipient plastic regime when dislocations are nucleated. Between these two regimes we report a novel one, in which dislocations nucleate at the steps but no pop-ins are visible. This novel regime is to a large extent reversible in the sense that defects disappear when the tip is retracted$^{[2]}$. Heterogeneous dislocation nucleation is catalyzed by the presence of the surface steps.


$^{[2]}$V. Navarro et al. Submitted

4:18PM L39.00008 Hysteresis in Kinking Nonlinear Elastic Solids and the Preisach-Mayergoz Model, PETER FINKEL, AICUO ZHOU, Drexel University, GARY FRIEDMAN, Drexel University, MICHEL BARSOUM, Drexel University — We show that the stress-induced, dislocation-based, elastic kypic loops of kinking nonlinear elastic solids – polycrystalline cobalt, Ti3SiC2 and a 10 vol. % porous Ti2AlC - obey the scalar Preisach-Mayergoz phenomenological model because they exhibit wipe-out and congruency, two necessary and sufficient tenets of the model. We also present experimental proof of the applicability of the model for the prediction of the response of these materials to complex stress histories.

4:30PM L39.00009 Strain Relaxation through Structural Phase Transition in Ultrathin Films of FCC Metals, KEDARNATH KOLLURI, M. RAUF GUNGOR, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report a computational analysis of atomistic mechanisms of relaxation of biaxially applied tensile strain over a broad range of strain levels, ε, in freestanding ultra-thin Cu films based on iso-thermal-iso-strain large-scale molecular-dynamics simulations. Our analysis reveals that for ε < 10%, plastic deformation occurs through ductile void growth and dislocation nucleation and glide from the thin-film surfaces. For ε > 10%, strain relaxation is dominated by the nucleation of a high density of dislocations at the film’s surface, leading to a martensitic transformation of the thin film from an fcc to a hcp lattice structure. The hcp phase nucleates at the surface of the thin film and propagates into the film due to the glide of dislocations; in this process, the relative atomic slips have magnitudes identical to those observed in Bain transformations. Furthermore, mechanical analysis according to generalized stability criteria shows that the observed phase transition is consistent with the onset of a shearing instability of the thin film.

4:42PM L39.00010 Mechanical Properties and Fracture of Electrochemically Deposited CdSe Nanocrystal Films, SHENGGuo JIA, SARBABIT BANERJEE, DONGyun Lee, JOZe BEvK, JEFFREY KYsAR, IRVING HERMAN, Materials Research Science and Engineering Center, Columbia University — The fracture, strain, and stress of electrochemically deposited (EPD) CdSe nanocrystal films are studied as a function of the film thickness, nanocrystal size, and drying method. Fracture results from the film stress that develops with the loss of residual solvent after EPD, when the film exceeds a threshold thickness. Generational crack formation and a preferred direction for film drying are observed in real time. The elastic modulus and hardness of films of 3.2 nm CdSe nanocrystals are studied as a function of the film thickness, nanocrystal size, and drying method. For ε < 10%, plastic deformation occurs through ductile void growth and dislocation nucleation and glide from the thin-film surfaces. For ε > 10%, strain relaxation is dominated by the nucleation of a high density of dislocations at the film’s surface, leading to a martensitic transformation of the thin film from an fcc to a hcp lattice structure. The hcp phase nucleates at the surface of the thin film and propagates into the film due to the glide of dislocations; in this process, the relative atomic slips have magnitudes identical to those observed in Bain transformations. Furthermore, mechanical analysis according to generalized stability criteria shows that the observed phase transition is consistent with the onset of a shearing instability of the thin film.

4:54PM L39.00011 Current-induced Stabilization of Surface Morphology in Stressed Solids, VIVEK TOMAR, M. RAUF GUNGOR, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report results on the surface morphological evolution of a conducting crystalline solid under the simultaneous action of an electric field and mechanical stress based on a fully nonlinear model and combining linear stability theory with self-consistent dynamical numerical simulations. Surface diffusional anisotropy is taken into account in the analysis. We address the evolution of a conducting crystalline solid under the simultaneous action of an electric field and mechanical stress based on a fully nonlinear model and combining linear stability theory with self-consistent dynamical numerical simulations. Surface diffusional anisotropy is taken into account in the analysis. We address the evolution of a conducting crystalline solid under the simultaneous action of an electric field and mechanical stress based on a fully nonlinear model and combining linear stability theory with self-consistent dynamical numerical simulations. Surface diffusional anisotropy is taken into account in the analysis. We address the evolution of a conducting crystalline solid under the simultaneous action of an electric field and mechanical stress based on a fully nonlinear model and combining linear stability theory with self-consistent dynamical numerical simulations. Surface diffusional anisotropy is taken into account in the analysis. We address the evolution of a conducting crystalline solid under the simultaneous action of an electric field and mechanical stress based on a fully nonlinear model and combining linear stability theory with self-consistent dynamical numerical simulations. Surface diffusional anisotropy is taken into account in the analysis.
and finally allowed to release isentropically. Here, we will discuss the details of the experiments and error analysis in deriving the yield strength of aluminum.

The aluminum samples were initially shocked to a fixed state on the Hugoniot, then quasi-isentropically compressed, to achieve a state of fixed entropy. The phase diagram. We employed these advances in recent tailored dynamic experiments to gain insight into the yield strength of aluminum along "hot" isentropes.

The formulation can be used in analyzing deformation mechanisms associated with defects involving heterogeneous fields at the nanoscale and macroscale, and in studying nanoscale processes where nonlocality is important.

We acknowledge support from NSF-DMR and DOE/NNSA (CDAC).

Work supported by the National Science Foundation.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344.
3:30PM L40.00006 Violation of the London law and Onsager–Feynman quantization in multi-component superconductors, EGOR BABAЕV, University of Massachusetts Amherst, NEIL W. ASHCROFT, Cornell University — Non-classical response to rotation is a hallmark of quantum ordered states such as superconductors and superfluids. The rotational responses of all currently known single-component ‘super’ states of matter (superconductors, superfluids and supersolids) are largely described by two fundamental principles and fall into two categories according to whether the systems are composed of charged or neutral particles: the London law relating the angular velocity to a subsequently established magnetic field and the Onsager–Feynman quantization of superfluid velocity. These laws are theoretically shown to be violated in a two-component superconductor such as the projected liquid metallic states of hydrogen and deuterium at high pressures. The rotational responses of liquid metallic hydrogen or deuterium identify them as a new class of dissipationless states; they also directly point to a particular experimental route for verification of their existence.

3:42PM L40.00007 Ab-initio study on the crystal structure and the superconductivity of calcium in phase IV and $\gamma$, TAKAHIRO ISHIKAWA, HITOSE NAGARA, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University, NAOSHI SUZUKI, Department of Pure and Applied Physics, Kansai University — Calcium shows interesting structural phase transitions and the superconductivity under high pressure. Structural transformations from the simple cubic structure (Ca-III) to a complex structure (Ca-IV) at 133GPa and from Ca-IV to another complex one (Ca-V) at 139GPa have been reported, but their structures have not been identified. The pressure-induced superconducting transition has been observed in Ca-III, and the superconducting transition temperature $T_c$ dramatically increases at the transition from Ca-III to Ca-IV and reaches to 25K, which is the highest $T_c$ in an element, at 161GPa in Ca-V. We explored the structures of Ca-IV and Ca-V via the metadynamics simulation based on the density functional theory and obtained two new structures: A helical structure and a zigzag structure. From comparison of the $x$-ray diffraction patterns we identified that the helical structure and the zigzag structure are candidate structures of Ca-IV and Ca-V, respectively. For the zigzag structure of Ca-V we calculated Tc using the Allen-Dynes formula. We assumed the effective screened Coulomb repulsion constant $\mu^*$ to be 0.1. We obtained $T_c=18.19$K at 140GPa, and the estimated values of $T_c$ are high and are close to the experimental values of Ca-V.

3:54PM L40.00008 Pressure-induced insulator-metal and structural transitions of BaBiO$_3$ from first principles LDA+$U$, DAVIDE CERESOLI, SISSA, Trieste, ERIO TOSATTI, SISSA and ICTP, Trieste — At zero pressure and temperature BaBiO$_3$ is an insulator with a structural dimerization, equivalent to a static valence disproportionation of the two Bi ions per cell from 4+ to 3+/5+. Under pressure one would expect an insulator-metal transition and the eventual disappearance of the dimerization. Moreover, the metallic phase should be superconducting, in analogy the metal doped Ba$_{1-x}$K$_{x}$BiO$_3$ compounds. To date, there are no accurate ab initio predictions under pressure, essentially because LDA or GGA fail to stabilize an insulating phase with the correct distortion and electronic gap. We carried out first principles LDA+$U$ calculations by determining the effective Hubbard U self-consistently at every pressure, and that the presence of U is mandatory for a correct description of the zero-pressure state. Upon increasing pressure, we found an insulator to metal transition at $\sim 20$ GPa. By further increasing the pressure, we predict the appearance of a superconducting phase, characterized by quantum melting of the weakly dimerized CDW lattice. The dimerization tendency and superconductivity are expected to weaken only at much higher pressures, presently under investigation.

4:06PM L40.00009 High pressure magnetic phase transitions in the quasi-2D ferromagnet, CeCrSb$_3$ investigated using designer diamond anvils, D.D. JACKSON, S.K. MCCALL, S.T. WEIR, Lawrence Livermore National Laboratory, A.B. KARKI, D.P. YOUNG, Louisiana State University, W. QIU, Y.K. VOHRA, University of Alabama, Birmingham — Pressure tuning magnetic phase transitions is a powerful method of discovering new physical properties of materials. At ambient pressure, CeCrSb$_3$ undergoes ferromagnetic ordering at 115 K due to the Cr ions, followed by a gradual ferromagnetic alignment of the Ce moments between 48 and 18 K. The evolution of these magnetic transitions was investigated via ac magnetic susceptibility to pressures of 20 GPa using designer diamond anvils. The ferromagnetic ordering due to the Cr ions decreases at a rate of $d T_c / d P = -1.75$ K/GPa, while the onset of the Ce ferromagnetic ordered phase increases at a rate of $d T_c / d P = 3.6$ K/GPa, followed by a sharp drop at $P_t = 11$ GPa. In addition, the electrical resistivity reveals that a possible superconducting phase is found between 11 GPa $< P < 16$ GPa below $T_t$ $\approx 3$ K.

4:18PM L40.00010 Zirconium Hydride: Structural Integrity at High-Pressures - A Synchrotron X-Ray Diffraction Study, PATRICIA E. KALITA, A. CORNELIUS, Department of Physics, University of Nevada Las Vegas, NV, USA, S. SINOGEIKIN, Geophysical Lab, Carnegie Institution of Washington, Washington DC, USA, A. MARTIN, Department of Physics, Xavier University of Louisiana, New Orleans, LA, USA, T. HARTMANN, Institute of Nuclear Science & Engineering, Idaho State University, Idaho Falls, ID 83401, USA, K.E. LIPINSKA-KALITA, Dept. of Chemistry, University of Nevada Las Vegas, NV, USA — Metal hydrides are of great interest not only from the fundamental research point of view but also because of their many technological applications, including hydrogen storage. Here we present our most recent studies in situ, high-pressure, angle-dispersive, synchrotron x-ray diffraction studies of zirconium hydride. We investigate the effects of hydrostatic and non-hydrostatic conditions. We also show the results of structural refinements as well as the bulk modulus of ZrH$_2$. *Work at UNLV is supported by DOE award No. DEFG36-07NA27344.

4:30PM L40.00011 Structural changes in borohydride hydrogen storage materials, RAVHI KUMAR, HiPSEC, Dep.Physics, University of Nevada Las Vegas, NV 89154, ANDREW CORNELIUS, HiPSEC, Department of Physics and Astronomy, University of Nevada Las Vegas, NV 89154, MALCOLM NICOL, HiPSEC, Department of Physics and Astronomy, University of Nevada Las Vegas, NV 89154 — Angle dispersive powder x-ray diffraction and Raman experiments were performed on ABH$_4$ ($A = K, Rb$) at high pressures up to 27 GPa. We demonstrate that KBH$_4$ exhibits structural phase transitions from the ambient $\alpha$-KBH$_4$ phase (cubic Fm-3m) to $\beta$-KBH$_4$ (tetragonal-P421c) at 3.8 GPa and to $\gamma$-KBH$_4$ phase (orthorhombic-Pnma) at 6.8 GPa which is similar to the phase transition sequence observed for NaBH$_4$ earlier [1]. However, RbBH$_4$ undergoes two successive pressure induced structural transitions from the ambient $\beta$-KBH$_4$ phase to an orthorhombic Pnma phase around 2.9 GPa and then to a monoclinic phase above 8 GPa. The high pressure monoclinic phase is found to be stable up to 27 GPa. The experimental results reveal the phase transition sequence exhibited by RbBH$_4$ is different from the pressure induced changes observed in similar cubic compounds NaBH$_4$ and KHBH$_4$. The results further show that both the transition pressure and the structural ordering at high pressures are influenced by the atomic size of the alkali cation in these compounds. [1]. R.S. Kumar and Andrew L. Cornelius, App.Phys.Lett., 2005, 87, 261916.

*Work at UNLV is supported by DOE award No. DEFG3605GO08502. HiPSEC is supported by DOE, NNSA under co-operative agreement DE-FC08-01NV14049.
Session P1 DCMP: Is There Pairing Glue in Cuprate Superconductors?

Wednesday, March 12, 2008 8:00AM - 11:00AM  
Session P1 DCMP: Is There Pairing Glue in Cuprate Superconductors?  
LaLouisiane AB

8:00AM P1.00001 The Question of Pairing Glue in the Cuprate Superconductors1, DOUGLAS SCALAPINO, UCSB — The Hubbard and t-J models exhibit many of the properties which are observed in the cuprate superconductors. Thus they provide a framework for addressing the question of whether one should expect to find a “pairing glue” in the cuprates. This question is basically a question regarding the dynamics of the pairing interaction. If the dynamics of the pairing interaction arises from virtual states, whose energies correspond to the Mott gap, and give rise to the exchange coupling J, the interaction is instantaneous on the relative time scales of interest. In this case one would not speak of a pairing glue. However, if the energies correspond to the spectrum seen in the dynamic spin susceptibility, then the interaction is retarded and one could speak of a spin-fluctuation glue which mediates the d-wave pairing interaction. We will review results from recent numerical calculations which provide insight into this question.

1Supported by NSF-DMR 0528969.

8:36AM P1.00002 Strongly Correlated d-wave Superconductivity: a CDMFT Perspective1, GABRIEL KOTLIAR, Rutgers University — We examine the impact of the proximity to a Mott insulating state on the superconducting properties of model new crystal structures previously unknown for these materials, of [0001] direction or uniaxial tension along the [110] direction, causes a transformation to a five-fold coordinated unbounded wurtzite structure which we named HX. On the other hand, uniaxial tension along the [0001] direction causes the materials to transform into a body-centered-tetragonal structure which we named BCT-4. The critical equilibrium transformation stresses for these transformations are obtained and their correlation with the ionicity of the materials is analyzed.

1Currently at CWRU, Cleveland, OH 44106.
9:12AM P1.00003 The Fluctuating Bond Model, a Glue for Cuprate Superconductivity? 1. DENNIS NEWNS, IBM T.J. Watson Research Center — Twenty years of research have yet to produce a consensus on the origin of high temperature superconductivity (HTS). The mechanism of HTS - which originates in the CuO₂ plane, common to all HTS families - can be constrained by some key experimental facts regarding superconducting and pseudogap behaviors. Superconductivity, involving a Tc of order 100K, exhibits an unusual d-wave superconducting gap, with Fermi liquid nodal excitations, and an anomalous doping-dependent oxygen isotope shift. A "pseudogap," also with d-symmetry, leads to a dip in the density of states below a characteristic temperature scale T*, which has a negative isotope shift; we associate the pseudogap with the recently observed spatially inhomogeneous (nanometer-scale) C₄ symmetry breaking. The isotope shifts and other evidence imply a key role for oxygen vibrations, but conventional BCS single-phonon coupling is essential for this purpose, and by the on-site Coulomb interaction U. In a novel approach, we introduce a model based on a strong, local, nonlinear interaction between electrons within the Cu-O-Cu bond in the CuO₂ plane, and the oxygen vibrational degrees of freedom, termed the Fluctuating Bond Model (FBM) [D.M. Newns and C.C. Tsuei, Nature Physics 3, 184 (2007)]. In mean field the model predicts a phase manifesting broken C₄ symmetry, with a d-type pseudogap, and an upper phase boundary in temperature, with a negative isotope shift, which we identify with T*. An intrinsic d-wave pairing tendency is found, leading to a transition temperature dome and an anomalous isotope shift similar to that found experimentally. The softening in the oxygen vibrational frequency below Tc, seen in Raman and neutron spectra, has a natural explanation in the FBM. Recent ab initio calculations have been implemented which provide microscopic support for the model.

1Work done with C.C. Tsuei.

9:48AM P1.00004 The Normal State Pseudogap in Underdoped Cuprates: Precursor Pairing vs. Competing Order? 1, MOHIT RANDERIA, The Ohio State University — The "pseudogap" in the normal state of underdoped High Tc cuprates refers to a set phenomenon associated with the loss of low energy spectral weight in various spectroscopies, starting at a temperature T*(x), much higher than Tc(x), and with a completely different doping dependence. Understanding the unusual phenomena in the pseudogap regime, which lies between the Mott insulator and the optimally doped superconductor, is an important challenge for any theory of high Tc superconductivity. I will first review some of the main experimental facts about the pseudogap, focusing in particular on recent angle-resolved photoemission (ARPES) data. I will then critically examine which aspects of the data can be qualitatively understood in terms of theories of precursor pairing or those based on a competing order parameter.

10:24AM P1.00005 Two-Dimensional Hubbard Model and High-Tc Superconductivity 1. MASATOSHI IMADA, University of Tokyo — No abstract available.

Wednesday, March 12, 2008 8:00AM - 9:48AM — Session P2 DCMP: Controlling Electron Spins: Propagation and Dynamics Morial Convention Center LaLouisiane C

8:00AM P2.00001 An Exact SU(2) Symmetry and Persistent Spin Helix in a Spin-Orbit Coupled System 1. B. ANDREI BERNEVIG, Princeton University — Spin-orbit coupled systems generally break the spin rotation symmetry. However, for a model with equal Rashba and Dresselhaus coupling constant (the ReD model), and for the [110] Dresselhaus model, a new type of SU(2) spin rotation symmetry is discovered. This symmetry is robust against spin-independent disorder and interactions, and is generated by operators whose wavevector depends on the coupling strength. It renders the spin lifetime infinite at this wavevector, giving rise to a Persistent Spin Helix (PSH). We obtain the spin fluctuation dynamics at, and away, from the symmetry point, and suggest experiments to observe the PSH. Recent experimental efforts have already discovered signs of the Persistent Spin Helix. Although reaching the Rashba equal to Dresselhaus point is difficult, the Persistent Spin Helix manifests itself in a long-lived spin-density wave even from this point, making its discovery especially suitable for optical techniques such as transient spin-grating spectroscopy. The SU(2) symmetric point allows one to obtain the exact analytic transport equations from the diffusive to the ballistic regime, which has previously been accessible only through numerical work.

8:36AM P2.00002 Evidence for a persistent spin helix in a 2-dimensional electron gas 1. JAKE D. KORALEK, LBNL and UC Berkeley — Using time-resolved transient spin-grating spectroscopy we uncover strong evidence for the existence of a persistent spin helix (PSH) in a 2-dimensional electron gas. The PSH is a collective helical spin excitation that persists far beyond the lifetime of its individual constituent spins when the Rashba (α) and Dresselhaus (β) spin-orbit coupling terms are comparable. The helix is predicted to have an infinite lifetime when they are exactly equal. These effects have great potential for application to spintronics where they would allow rapid control of the spin lifetime over several orders of magnitude in systems with both high electron density and high mobility. The transient spin-grating technique is ideally suited for study of the PSH as it can directly measure the dynamics of optically generated spin excitations of variable spatial periodicity. This is accomplished by interfering two non-collinear, orthogonally polarized pulses from a Ti:Sapphire laser at the surface of the sample. Through the optical orientation effect in GaAs, this generates a spin excitation which varies periodically in space between up and down spins at a wavelength determined by the angle between the interfering pulses. We tune the spin-orbit coupling in our GaAs based quantum wells through asymmetric modulation doping, which has allowed us to increase a to be comparable to β. In these systems we find that spin-gratings with periodicity comparable to that of the PSH can live several orders of magnitude longer than the individual spin lifetime as measured by time-resolved Faraday rotation. We study this over a wide range of parameter space, systematically varying doping asymmetry, well width, and disorder. We find that the lifetime of the PSH in these samples is ultimately limited by the spatial disorder in the Rashba strength, and by a novel relaxation mechanism based on phonon-induced Rashba coupling. Supported by DMSE office of BES-DGE, NSF, MARCO, ASEE and CNID.

1In collaboration with C.P. Weber and J. Orenstein, LBNL and UC Berkeley, S. Mack and D.D. Awschalom, CSQC and UC Santa Barbara.
change, mechanics will also consider briefly the influence of diffusion on aggregation properties. Our understanding of dynamical properties close to the sol-gel transition is lower as another important concept also introduced by de Gennes concerning the possibility of observation of classical exponents in the case of vulcanization. We made by de Gennes and Stauffer. We will discuss some recent experiments showing the relevance of percolation in the description of the sol-gel transition, as because both excluded volume interactions and loops were neglected. An important progress was made when an analogy between percolation and gelation was proposed as the basis of micro-actuation and artificial muscles, both heat and light-driven. In 1969, de Gennes already described ideal networks heated through Morial Convention Center 206.

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P3 DPOLY: Simple Views on Bulk Polymers: Symposium Honoring P G de Gennes

8:00AM P3.00001 How Polymer Physics Was Born, PHILIP PINCUS, Physics Department, UCSB — We review the physics of some of de Gennes’ principal contributions to fundamental aspects of polymer solution science. These include critical phenomena views on interacting polymers, reptation, polyelectrolytes, and gels.

8:36AM P3.00002 Polyelectrolyte Solutions, RALPH H. COLBY, Materials Science and Engineering, Penn State University — Pierre-Gilles de Gennes once described polyelectrolytes as the “least understood form of condensed matter”. In this talk, I will describe the state of the polyelectrolyte field before and after de Gennes’ seminal contributions published 1976-1980. De Gennes clearly explained why electrostatic interactions only stretch the polyelectrolyte chains on intermediate scales in semidilute solution (between the electrostatic blob size and the correlation length) and why the scattering function has a peak corresponding to the correlation length (the distance to the next chain). Despite many other ideas being suggested since then, the simple de Gennes scaling picture of polyelectrolyte conformation in solution has stood the test of time. How that model is used today, including consequences for dynamics in polyelectrolyte solutions, and what questions remain, will clarify the importance of de Gennes’ ideas.

9:12AM P3.00003 Block Copolymers, LUDVIK LEIBLER, Matière Molle et Chimie, UMR 7167 CNRS/ESPCI, ESPCI, 10 rue Vauquelin, 75005 PARIS, France — In 1969 (Rep. Prog. Phys. 32, 187(1969)) de Gennes proposed a simple way to understand and describe mesophase organization of block copolymers in what we now call the strong segregation limit. The following year he showed how self-consistent methods due to Edwards can be applied to understand subtle correlation effects in polymer melts (J. Physique 31, 235(1970)) and established theoretical framework for quantitative interpretation of scattering experiments and of what we call now weak segregation regime of block copolymers. This was the basis of the theory of order-disorder transition in multiblock copolymers that he published in 1980 (Faraday Transactions). In this pioneering work he also discussed the role of blocks’ polydispersity. Eventually, as early as in 1977 de Gennes realized that block copolymers “are most promising systems for deeper understanding of lyophilic phase diagrams” (in Suppl. Solid State Phys Ed. Ehrenreich 1977) and this vision led not only to some very interesting theories of block copolymer solutions, but also to some very quantitative model of membranes and interfaces elasticity and to a very influential theory of microemulsions (J. Phys. Chem. 86, 2294(1982)). Since 1980 tens of thousands of papers dealing with block copolymers were published, but it should be stressed that in seventies it has been a very unknown area. Clearly de Gennes’ visionary block copolymer research has had a very important impact in the field. I will illustrate using several examples from very different areas how de Gennes’ deep understanding of block copolymers and the theoretical methods he introduced influenced both theory and experiments and I will also show how they are relevant for many present and future industrial applications.

9:48AM P3.00004 Percolation and Gelation, MOHAMED DAOUD, CEA Saclay — The sol-gel transition, as well as the vulcanization of Polymers chains, was described long ago by Flory, Stockmayer, Zimm within mean field approximation. This however had strong limitations because both excluded volume interactions and loops were neglected. An important progress was made when an analogy between percolation and gelation was made by de Gennes and Stauffer. We will discuss some recent experiments showing the relevance of percolation in the description of the sol-gel transition, as well as another important concept also introduced by de Gennes concerning the possibility of observation of classical exponents in the case of vulcanization. We will also consider briefly the influence of diffusion on aggregation properties. Our understanding of dynamical properties close to the sol-gel transition is lower than that of the static ones. Some analogies were given by de Gennes to describe various hydrodynamic limits, but the experimental results still lead to some discussions. Finally, we will mention some generalizations and open questions.

10:24AM P3.00005 Liquid Crystalline Polymers and Networks — orientation, molecular shape change, mechanics, MARK WARNER, University of Cambridge — In a prescient paper of 1969, Pierre-Gilles de Gennes envisaged both liquid crystal polymers and elastomers. 10 years later, these systems were realised. After 25 years, monodomain elastomers were prepared and displayed phenomena he had predicted: rods incorporated into polymers induce liquid crystallinity in polymer melts and elastomers; orientational order causes shape changes in the backbone of such polymers; mechanical ramifications follow in networks, e.g. spontaneous elongations and contractions on changing order. The latter are proposed as the basis of micro-actuation and artificial muscles, both heat and light-driven. In 1969, de Gennes already described ideal networks heated through the nematic-isotropic transition losing all their order by mechanical relaxation. It is not obvious, but is true in theory and largely in experiment, even in highly non-ideal networks. He also envisaged that a cholesteric network, where there is a topological memory of chirality imprinted by crosslinking chains in a twisted state, chirality cannot relax away on entering the isotropic phase, even in systems without molecular chirality (for instance those crosslinked in the presence of chiral solvent that is subsequently exchanged away). His chiral elastomers have found application as mechanically-tunable, rubber lasers. De Gennes also constructed the first continuum elastic theories of nematic elastomers (1982), though distortions are generally very large. His elasticity has informed non-linear elasticity that works even at large amplitudes. I shall describe de Gennes’ many contributions, and the current state of a field that has since yielded still more remarkable phenomena.

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P4 GSNP: Fluctuations and Rare Events in Physical, Chemical, and Biological Systems

Morial Convention Center 206
8:00AM P4.00001 Rare events and phase transitions in reaction-diffusion systems

ALEX KAMENEV, University of Minnesota — I shall discuss a way to evaluate tails of the probability distribution functions in stochastic reaction-diffusion models. The method is based on the semi-classical treatment of a proper "quantum" field theory, which may be associated with reaction-diffusion systems. The same set of ideas may be applied to a classification of non-equilibrium phase transitions, taking place in these models. V. Elgart and A. Kamenev, Classification of phase transitions in reaction–diffusion systems, Phys. Rev. E 74, 041101 (2006). V. Elgart and A. Kamenev, Rare Events Statistics in Reaction–Diffusion Systems, Phys. Rev. E 70, 041106 (2004).

1Support of NSF Grant No. DMR 0405212 is greatly acknowledged.

8:36AM P4.00002 Switching and phase transitions in a parametrically-excited cold atom trap

WONHO JHE, Seoul National University — Stochastic dynamics of cold atoms in a modulated magneto-optical atom trap was investigated. The studies focused on the phenomenon related to switching between the parametrically excited period-2 states. The rates of single-atom activated transitions were analyzed. When the atom density was increased, there were observed Ising-class phase transitions where the symmetric population of period-2 states was spontaneously broken [1,2]. Anomalous fluctuations in the decay of the unstable state were investigated [3].


This work was supported by the Creative Research Initiative of Korea.

9:12AM P4.00003 Activation barrier scaling and switching path distribution in a micromechanical parametric oscillator

H.B. CHAN, University of Florida — Parametrically modulated systems develop multiple coexisting states under sufficiently large drive. In the presence of fluctuations, the system can occasionally overcome the activation barrier and switch from one state to the other, resulting in the phase of oscillation slipping by \( \pi \). We study noise-induced switching in a parametrically-driven micromechanical torsional oscillator. Certain properties of the switching are generic to bistable systems, while others are specific to nonequilibrium systems that lack detailed balance. For instance, close to the bifurcation points, the activation barrier for switching is expected to display system-independent scaling. By measuring the rate of random transitions at different fluctuation intensities, we deduce the activation barrier as a function of frequency detuning from the bifurcation points and measure a critical exponent that is in good agreement with theoretical predictions. We also measure the escape trajectories followed by the oscillator, confirming the notion that they form narrow tubes in phase space centered at the most probable escape path. The uphill section of this path is found to be distinct from its time-reversed downhill section, an important property for systems far from thermal equilibrium. Near the saddle point the velocity is significantly diminished and the motion becomes diffusive, leading to strong broadening and increase in height of the probability distribution. Apart from fundamental interest, the sharp change in the oscillation amplitude near the subcritical bifurcation point can provide accurate determination of device parameters.


BARUCH MEERSON, Hebrew University of Jerusalem — Statistics of rare events, or large deviations, in chemical reactions and systems of birth-death type have attracted a great deal of interest in many areas of science including cell biochemistry, astrochemistry, epidemiology, population biology, etc. Large deviations become of vital importance when discrete (non-continuum) nature of a population of "particles" (molecules, bacteria, cells, animals or even humans) and stochastic character of interactions can drive the population to extinction. I will briefly review the novel spectral method [1-3] for calculating the extreme statistics of a broad class of birth-death processes and reactions involving a single species. The spectral method combines the probability generating function formalism with the Sturm-Liouville theory of linear differential operators. It involves a controlled perturbative treatment based on a natural large parameter of the problem: the different fluctuation intensities, we deduce the activation barrier as a function of frequency detuning from the bifurcation points, the activation barrier for switching is expected to display system-independent scaling. By measuring the rate of random transitions at different fluctuation intensities, we deduce the activation barrier as a function of frequency detuning from the bifurcation points and measure a critical exponent that is in good agreement with theoretical predictions. We also measure the escape trajectories followed by the oscillator, confirming the notion that they form narrow tubes in phase space centered at the most probable escape path. The uphill section of this path is found to be distinct from its time-reversed downhill section, an important property for systems far from thermal equilibrium. Near the saddle point the velocity is significantly diminished and the motion becomes diffusive, leading to strong broadening and increase in height of the probability distribution. Apart from fundamental interest, the sharp change in the oscillation amplitude near the subcritical bifurcation point can provide accurate determination of device parameters.


This work was partially supported by awards NSF DEB-0328267 and NSF/NIH DMS/NIGMS-0342388.

10:24AM P4.00005 Strong Fluctuations and Cycling in Biological Systems

TIMOTHY NEWMAN, Arizona State University — In this talk I describe a mechanism for generating cycles in a large class of "mesoscale" biological populations (meaning populations composed of thousands to tens of thousands of units). Cycles are caused by a resonant amplification of the system dynamics triggered by internal noise. I will discuss this mechanism in the context of two classes of simple systems: ecological (e.g. predator-prey, host-pathogen) and biochemical (e.g. small gene regulation networks, modules of metabolic processes). [Predator-Prey Cycles from Resonant Amplification of Demographic Stochasticity, A. J. McKane and T. J. Newman, Physical Review Letters 94, 218102 (2005); Amplified Biochemical Oscillations in Cellular Systems, A. J. McKane, J. Nagy, T. J. Newman, and M. Stefanini, Journal of Statistical Physics 128, 165-191 (2007)].

Wednesday, March 12, 2008 8:00AM - 11:00AM – Session P5 GQI: Quantum Information Meets Gravitation Morial Convention Center R01

8:00AM P5.00001 Quantum Computational Complexity in the Presence of Closed Timelike Curves

DAVE BACON, University of Washington — What are the consequences of modifying the laws of physics for the theory of computation? Considering this question in the context of quantum theory has led to a seemingly new class of computing devices known as quantum computers. In this talk I will discuss how modifying computation (in a quantum or classical context) to allow for closed timelike curves leads to a new model of computation. In particular I will discuss how such a model of computation with closed timelike curves can be formulated, whether it can be made robust to noise, and how recent results of Aaronson and Watrous show that this model is no more than the well studied complexity class PSPACE. Consequences of these results on foundational issues in quantum theory will also be discussed.
8:36AM P5.00002 Black holes as mirrors: quantum information in random subsystems, JOHN PRESKILL, Caltech — We study information retrieval from evaporating black holes, assuming that the internal dynamics of a black hole is unitary and rapidly mixing, and assuming that the retriever has unlimited control over the emitted Hawking radiation. If the evaporation of the black hole has already proceeded past the “half-way” point, where half of the initial entropy has been radiated away, then additional quantum information deposited in the black hole is revealed in the Hawking radiation very rapidly. Information deposited prior to the half-way point remains concealed until the half-way point, and then emerges quickly. These conclusions hold because typical local quantum circuits are efficient encoders for quantum error-correcting codes that nearly achieve the capacity of the quantum erasure channel. Our estimate of a black hole’s information retention time, based on speculative dynamical assumptions, is just barely compatible with the black hole complementarity hypothesis. This is joint work with Patrick Hayden.

9:12AM P5.00003 Entanglement in non-inertial frames and curved spacetime, IVETTE Fuentes-Schuller, University of Potsdam, Germany — The insight that the world is fundamentally quantum mechanical inspired the development of quantum information theory. However, the world is not only quantum but also relativistic, and indeed many implementations of quantum information tasks involve truly relativistic systems. In this talk I consider relativistic effects on entanglement in flat and curved spacetimes. I will emphasize the qualitative differences to a non-relativistic treatment, and demonstrate that a thorough understanding of quantum information theory requires taking relativity into account. The exploitation of such relativistic effects will likely play an increasing role in the future development of quantum information theory. The relevance of these results extends beyond pure quantum information theory, and applications to foundational questions in cosmology and black hole physics will be presented.

9:48AM P5.00004 Spin-induced non-geodesic motion, Wigner rotation and EPR correlations of massive spin-1/2 particles in a gravitational field1, PAUL M. ALSING, University of New Mexico — We investigate in a covariant manner, the spin-induced non-geodesic motion of massive spin-1/2 particles in an arbitrary gravitational field for trajectories that are initially geodesic when spin is ignored. Using the WKB approximation for the wave function in an arbitrary curved spacetime, we compute the $O(\hbar)$ correction to the Wigner rotation of the spin-1/2 particle, whose $O(1)$ contribution is zero on timelike geodesics. We consider specific examples in the Schwarzschild metric for motions in the equatorial plane for (i) particles falling in from spatial infinity with non-zero angular momentum and (ii) circular geodesic orbits. For the latter case we consider the Bell inequalities for a perfectly anti-correlated EPR entangled pair of spins as the separate qubits traverse the circular geodesic in opposite directions.

1 In collaboration with G.J. Stephenson Jr., University of New Mexico and Patrick Kilian, Universitat Wuerzburg, Germany.

10:24AM P5.00005 Quantum Graphity: a model of emergent locality, FOTINI MARKOPOULOU, Perimeter Institute for Theoretical Physics — Quantum graphity is a background independent condensed matter model for emergent locality, spatial geometry and matter in quantum gravity. The states of the system are given by bosonic degrees of freedom on a dynamical graph on N vertices (that is, changing in time). At high energy, the graph is the complete graph on N vertices and the physics is invariant under the full symmetric group acting on the vertices and highly non-local. We find evidence that the model has a phase, in which the ground state breaks the permutation symmetry to translations and discrete rotations. In this phase the system is ordered, low-dimensional and local. Consideration of the free energy associated with the dominant terms in the dynamics shows that the ground state is thermodynamically stable under local perturbations. The model gives rise to an emergent U(1) gauge theory in the ground state by the string-net condensation mechanism of Levin and Wen. We will reformulate the model in graph-theoretic terms and compare its dynamics to some common graph processes.

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P6 DFD: Fluid Dynamics and Biology Morial Convention Center RO4

8:00AM P6.00001 Depolymerization-driven flow and the crawling of nematode sperm, CHARLES WOLGEMUTH, UCONN Health Center — Cell crawling motility is integral in many biological and biomedical processes, such as wound healing, cancer metastasis, and morphogenesis. A complete understanding of the mechanics by which cells crawl is still lacking, but it is known to entail at least three separate physical processes: (i) cytoskeletal extension at the front of the cell; (ii) adhesion to the substrate at the cell front and release at the rear; and (iii) advance of the cell body. In most cells, the cytoskeletal network is composed of actin. The mechanism by which force is generated to drive translocation of the cell body is still debated. Originally, this force was attributed to an actomyosin system similar to muscle. However, nematode sperm utilize a cytoskeleton composed of a network of Major Sperm Protein (MSP) that forms non-polar filaments for which molecular motors have not been identified. The motility of these cells still exhibits all three fundamental processes required for standard crawling motility. Experiments suggest that depolymerization of the cytoskeletal network is the force-producing mechanism for pulling up the rear. In this talk I will present a mechanical model that describes how depolymerization of the cytoskeleton can drive motility. This model accounts for both cytoskeletal displacements and cytosolic (the fluid component of the cell) flow. The model accurately fits in vitro data using nematode sperm extracts where depolymerization induces contraction of MSP polymer bundles. Application of this model to cell crawling produces testable predictions about how the size and shape of a cell affect crawling speed. Experiments using Caenorhabditis elegans sperm show good agreement with the model predictions. Interestingly, the model requires that cells are anisotropically elastic, being more stiff in the direction of motion perpendicular to it. A simple physical picture can account for this anisotropy. The model also predicts that cell speed increases with anisotropy and with depolymerization rate.

8:36AM P6.00002 Optimizing Low Reynolds Number Locomotion, ANETTE HOSOI, MIT — In this talk I will discuss optimal stroke patterns for low Reynolds number linked swimmers. We begin by optimizing stroke patterns for Purcell’s 3-link swimmer modeled as a jointed chain of three slender links moving in an inertialless flow. The swimmer is optimized for efficiency and speed and we are able to attain significant increases is efficiency over those previously suggested by authors who only consider geometric design rather than kinematic criteria. We then go on to investigate unflagellate and biflagellate organisms and compare the optimized results to biological data from spermatozoa and chlamydomonas.
On ultracold Fermions and Bose-Fermi mixtures in optical lattices will be presented. A "Coulomb-blockade" type tunnelling resonance one can count atoms one by one to determine their number statistics in the lattice potential. Finally, latest such superexchange interactions for the investigation of dynamical behaviour in quantum spin systems and for quantum information processing will be outlined.

In optical superlattices in an antiferromagnetically ordered state, we are able to observe a coherent superexchange mediated spin dynamics down to coupling measurement of such superexchange interactions with ultracold atoms in optical lattices. After preparing a spin-mixture of ultracold atoms with the help of magnetism in strongly correlated electronic media and are believed to play a major role in high-Tc superconducting materials. We report on the first direct realization of super-exchange interactions in ultra-cold atoms. The many-body dynamics arising from the coherent coupling between singlet-triplet pairs in adjacent double-wells will be also discussed. In particular, we will describe how it can lead to the formation of frustrated spin states with a high degree of density fluctuations, which appear to be driven by the active stress instability.

This work is in collaboration with Michael Shelley (NYU)

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**Life in a drop of Ocean: microfluidic insights into microbial ecology**

ROMAN STOCKER, Civil and Environmental Engineering - MIT — Bacteria are the most abundant and successful form of life on Earth. Their physico-chemical interactions with their fluid environment are surprisingly complex and have enormous implications, which we can only hope to grasp if we learn to study microorganisms within realistic microenvironments. Microfluidics for the first time enables us to create microhabitats, including chemical and fluid mechanical landscapes, while visualizing bacterial behavior at a single-cell resolution. Here I focus on the application of microfluidics to gain insight in the life of marine bacteria. In their quest for nutrients, marine bacteria often experience the Ocean as a desert, where rare and ephemeral nutrient patches represent transient resource oases. In this patchy seascape, swimming and chemotaxis represent critical assets, but effective patch utilization is constrained by energetic requirements. And then there are predators and viruses... These interactions form the basis of the ‘microbial loop’, the ensemble of microbial processes known to directly impact the productivity of marine ecosystems and the rates of carbon turnover in the Ocean. I will show how fundamental new insight on selected aspects of microbial life in a drop of Ocean can be achieved by a combination of microfluidic experiments and theoretical modeling.

1 We acknowledge support from the NSF Division of Mathematical Sciences

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**Optimal flexibility in flapping appendages**

SILAS ALBEN, Georgia Institute of Technology — When oscillated in a fluid, appendages such as insect wings and fish fins can produce large thrust forces while undergoing considerable bending. Can we understand these bending patterns by comparing them with the patterns which produce maximum thrust, or a given thrust at maximum efficiency? We present a general model for how flexible surfaces produce vorticity and bend actively and passively in a fluid. We solve the model numerically, and discuss results for moderate deflections (relevant for large thrust), and for small deflections (relevant for high efficiency). We’ll then consider how a fish-fin-like structure might be designed for optimal performance.

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**Repulsively bound atom pairs in an optical lattice**

JOHANNES HECKER DENSCHLAG, Experimentalphysik, Universitaet Innsbruck — Three dimensional optical lattices represent an interesting environment for fundamental research with ultracold atoms. We have observed novel kind of stable bound state of two atoms which is based on repulsion rather than attraction between the particles [1]. We will explain how these lattice-induced repulsively bound pairs can be used to study strongly correlated condensed matter physics. [1] K. Winkler et al., Nature 441, 853 (2006).

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**Critical velocity for superfluid flow across the BEC-BCS crossover**

DANIEL MILLER, Massachusetts Institute of Technology — Critical velocities have been observed in an ultracold superfluid Fermi gas throughout the BEC-BCS crossover. A pronounced peak of the critical velocity at unitarity demonstrates that superfluidity is most robust for resonant atomic interactions. Critical velocities were determined from the abrupt onset of dissipation when the velocity of a moving one-dimensional optical lattice was varied. The dependence of the critical velocity on lattice depth and on the inhomogeneous density profile was studied.

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**Towards Quantum Magnetism with Ultracold Quantum Gases in Optical Lattices**

IMMANUEL BLOCH, Johannes Gutenberg Universität Mainz — Quantum mechanical superexchange interactions form the basis of quantum magnetism in strongly correlated electronic media and are believed to play a major role in high-Tc superconducting materials. We report on the first direct measurement of such superexchange interactions with ultracold atoms in optical lattices. After preparing a spin-mixture of ultracold atoms with the help of optical superlattices in an antiferromagnetically ordered state, we are able to observe a coherent superexchange mediated spin dynamics down to coupling energies as low as 5 Hz. Furthermore, it is shown how these superexchange interactions can be fully controlled in magnitude and sign. The prospects of using such superexchange interactions for the investigation of dynamical behaviour in quantum spin systems and for quantum information processing will be outlined in the talk. In addition we present results on the dynamical resolved co-tunnelling of repulsively bound atom pairs in optical superlattices and show how by using "Coulomb-blockade" type tunnelling resonance one can count atoms one by one to determine their number statistics in the lattice potential. Finally, latest results on ultracold Fermions and Bose-Fermi mixtures in optical lattices will be presented.

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**Probing and controlling quantum magnetism with ultra-cold atoms**

ANA MARIA REY, ITAMP — By loading spinor atoms in optical lattices it is now possible to experimentally implement quantum spin models. These systems allow the investigation of quantum magnetism in strongly correlated systems within a controlled environment. In this talk we will describe a novel approach to prepare, detect and control superexchange interactions in ultra-cold spinor atoms in optical superlattices [1]. Recently this approach was used for the first experimental realization of super-exchange interactions in ultra-cold atoms [2]. The many-body dynamics arising from the coherent coupling between singlet-triplet pairs in adjacent double-wells will be also discussed. In particular, we will describe how it can lead to the formation of frustrated spin states with a high degree of multi-particle entanglement. Finally, we will present an extension of this approach to prepare and detect d-wave pairing in an array of coupled plaquettes.


10:24AM P7.00005 Heteronuclear Molecules in a 3D Optical Lattice. CHRISTIAN OSPELKAUS, National Institute of Standards and Technology, 325 Broadway, Boulder, CO 80305, USA and Institut fuer Laser-Physik, Universitaet Hamburg, Germany — The production of ultracold polar molecular samples is a long standing goal of AMO and ultracold physics. The interest is motivated by novel quantum gases with anisotropic interactions between these polar molecules, by applications in quantum computation and simulation which benefit from the long-range interaction as well as by perspectives of measuring a T-violating permanent electric dipole moment of the electron in such a polar molecular system. While a lot of work has been done on direct cooling of polar molecules, a second proposed route to the production of ultracold polar molecules starts with ultracold atomic samples, where tremendous progress has been made in recent years, and assembles an ultracold atom mixture into weakly bound heteronuclear Feshbach molecules. These could then be transferred into the absolute internal molecular ground state using coherent Raman schemes. As a crucial step in this approach, we report where tremendous progress has been made in recent years, and assembles an ultracold atom mixture into weakly bound heteronuclear Feshbach molecules. The molecules are associated from a quantum degenerate mixture of fermionic $^{85}$Rb and bosonic $^{133}$Rb atoms loaded into a 3D optical lattice. The binding energy of the heteronuclear molecules is precisely determined by rf spectroscopy and compared to a theoretical model based on a pseudopotential approach. We also characterize both the lifetime of the sample and the efficiency of rf association; comparison to the pseudopotential model results in excellent agreement.

Wednesday, March 12, 2008 8:00AM - 11:00AM – Session P8 DFD: Glassy Dynamics Morial Convention Center R06

8:00AM P8.00001 Nonlinear Dynamics Near the Jamming Transition. EDWARD J BANIGAN, Dept of Physics and Astronomy, Univ of Pennsylvania, DAVID A EGOLF, Department of Physics, Georgetown University — How dynamical behaviors and static measures are related near the jamming transition remains an open question. In simulations of a two-dimensional sheared granular cell, we have calculated mathematical quantities that characterize the underlying nonlinear dynamics near the jamming transition. We find that the Lyapunov exponents and vectors characterizing the most important dynamical modes correlate well in space and time to localized events that alter the physical characteristics of the system. For example, the Lyapunov exponents and vectors highlight areas in which particles are involved in cooperative rearrangement or the formation or destruction of stress chains. In at least some cases, the behavior of the dynamical quantities appears to indicate future position or stress rearrangements. In addition, we report measurements of a dynamical time scale and a dynamical length scale that diverge as the system jams, suggesting an intriguing connection between the jamming transition and a transition between chaotic and non-chaotic dynamical states.

8:12AM P8.00002 Probing Cooperative Motion in Super-Cooled Colloidal Suspensions. PRASAD SARANGAPANI, Y. ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, 182 Fitzpatrick Hall, Notre Dame, IN 46556 — The physics of the glass transition remains inadequately understood despite its broad technological relevance. The anomalous divergence of viscosity without apparent structural change as a liquid is cooled has been attributed to the existence of growing dynamic length scales of “cooperatively rearranging regions” (CRR). In this work, we use ultra-fast fluorescence correlation spectroscopy (FCS) combined with high-speed imaging to determine the CRR sizes by measuring single-particle dynamics of tracer nano-particle embedded in super-cooled “hard-sphere” colloidal suspensions. Fluorescent poly-(methyl methacrylate) (PMMA) tracer particles of radii ranging from $r = 0.1-0.4 \mu m$, mixed with plain PMMA particles of radius, $r = 0.6 \mu m$ and bulk volume fraction, $\phi = 0.38-0.58$, serve as excellent probes for changes in the energy barrier landscape of the suspensions of increasing volume fraction and are sensitive to the creation and annihilation of isosahedral order in metastable colloidal fluids. We also find that the correlation length, determined by fluctuation-dissipation relations from the measured auto-correlation functions, shows a dramatic increase in the super-cooled regime until it diverges at $\phi = 0.58$.

8:24AM P8.00003 Structural relaxation in sheared two-dimensional foams. MATTHIAS MOBIUS, GJS KATGERT, MARTIN VAN HECKE, University of Leiden — Athermal and disordered systems at rest, such as foams and granular media, are stuck in a metastable configuration. Upon shear the system unjams and complex vortex-like rearrangements ensue that are correlated in time and space. In our experiment we investigate what the typical time scales of these structural relaxations are as a function of the local shear rate in a two-dimensional, disordered foam that is linearly sheared. After an initial super-diffusive regime, the bubbles become diffusive at later times. This transition is reflected in the statistics of the bubble displacements, which are initially strongly correlated and non-Gaussian but eventually become Gaussian. We find that the relaxation time decreases with shear rate. For large shear rates the dependence follows a power law with an exponent significantly different from -1.

8:36AM P8.00004 From spontaneous to induced dynamic fluctuations: Granular packings as an experimental probe. FREDERIC LECHENAULT, North Carolina State University, OLIVIER DAUCHOT, SPEC, CEA France, GIULIO BIROLI, SPHT, CEA France, JEAN-PHILIPPE BOUCHAUD, Science & Finance, Capital Fund Management — We track the motion of a horizontally vibrated amorphous assembly of bidisperse hard disks, for densities ranging across the jamming transition. The spatial extension of dynamical heterogeneities and the associated relaxation time are found to exhibit critical behavior. Moreover, a dynamical fluctuation inequality relating the dynamical susceptibility $\chi_d$ and the response of the dynamics to a change in density is tested. As the diffusion length is found to rescale these quantities, the dependencies of the inequality on length and time scales as well as density can be evaluated independently. Surprisingly, the lower bound is found to reproduce the non-monotonic behavior of $\chi_d$ in time, which reveals an intimate link between dynamical heterogeneity and marginal super diffusion. Finally, the bound is shown to be tight and to mimic the anomalous features of the dynamical susceptibility across the transition.

8:48AM P8.00005 Influence of the microstructure on jammed packings of spheres. ERIC CORWIN, MAXIME CLUSEL, ALEXANDER SIEMENS, JASNA BRUJIC, New York University — Jammed matter is by definition impenetrable to light, such that little is known about the geometry of jammed systems. Using confocal microscopy to image an emulsion in 3D, we use the enhanced fluorescence at the droplet contacts to determine the contact network inside this model frictionless system. This enables the experimental determination of the average coordination number $< Z >$, which agrees with the isostatic predicted value of $< Z > \approx 6$ [1]. Furthermore, we measure the distribution of coordination numbers within the jammed packings close to the isostatic limit. We show that the distribution of sizes of the droplets strongly influences the coordination number distribution, as well as the volume fraction at which the system becomes jammed. This may have important consequences on the stress propagation properties of the material as a whole. [1] J. Brujic et al., Phys. Rev. Lett. 98, 248001 (2007)

9:00AM P8.00006 Mode-coupling and generalized mode-coupling theory: a diagrammatic approach. GRZEGORZ SZAMEL, Department of Chemistry, Colorado State University — We present a diagrammatic approach to the dynamics of interacting Brownian particles. Within this approach, the time-dependent density correlation function is represented by a series of diagrams with three and four leg vertices. We analyze the structure of this series and obtain a diagrammatic interpretation of reducible and irreducible memory functions. The one-loop self-consistent approximation for the latter function coincides with mode-coupling approximation for Brownian systems that was derived previously using a projection operator approach. Finally, we investigate the diagrammatic interpretation of a generalized mode-coupling theory.
9:12AM P8.00007 Percolating Clusters in Systems of Gapped Rigid Rings, Christopher Lasota, Ariel Helper, Kenyon College — We have examined the behavior of kinetically agitated collections of rigid rings with angular gaps in them. For small gap angles, large clusters form readily and are sufficiently tangled so that they may be raised vertically under gravitational stresses without decomposing. Using gravity as a stressor under semi-static conditions, we have measured average cluster size as a function of the gap angle and witness what appears to be a second order percolation phase transition. The critical gap angle depends somewhat on the relative thickness of the ring material compared to the ring diameter. Although friction is necessary for the formation of clusters, it appears that cluster formation is dominated by geometry effects.

9:24AM P8.00008 Jamming transition in a temperature-sensitive 2D colloidal suspension, Zheng Zhang, Daniel T. N. Chen, Arjun G. Yodh, University of Pennsylvania, Kevin B. Aptowicz, West Chester University, Piotr Habdas, Saint Josephs University — We experimentally investigate the jamming transition of a 2D colloidal system. The system consists of a bidisperse mixture of thermo-responsive microgel particles confined between two glass slides, with a thickness of roughly the diameter of the larger particle. The packing density of the system is tuned by changing the temperature. A range of packing densities, both below and above the jamming transition is studied. We use video microscopy and particle tracking techniques to characterize the motion of the particles. On approaching the jamming transition the motion becomes slower and more heterogeneous. We characterize the jamming transition in terms of both structure (pair correlation function) and dynamics (mean square displacement, non-Gaussian parameter, four-point susceptibility). To our knowledge this study provides the first experimental evidence for the jamming transition in a 2D colloidal system.

9:36AM P8.00009 Exact Enumeration of Jammed States for Confined Hard Discs, S.S. Ashwin, Department of Chemistry, University of Saskatchewan, Richard K. Bowles, Department of Chemistry, University of Saskatchewan — Enumeration of jammed states of particle systems interacting with hard potentials such as hard discs and hard spheres is a long-standing problem which holds the key to understanding the nature of glassy dynamics and the question of the possibility of an ideal glass transition in these systems. A simple model consisting of hard discs (of diameter \( \sigma \)) trapped between two hard lines separated by a distance \( \beta ! \) exhibits slow relaxation and heterogeneous dynamics characteristic of glassy systems. We map the locally jammed structures in this model to tiles and pose the problem of enumeration of jammed states for the case \( H < 2\sigma \), as a tiling problem on a subset of a plane. Further on applying constraints for collective jamming on the arrangement of the tiles, we exactly enumerate the entire jamming landscape of the system and explore how this landscape is connected to the thermodynamics and dynamics of the glassy system.

We would like to thank NSERC and CFI for funding.

9:48AM P8.00010 Heterogeneities in granular dynamics, Anita Mehta, S. N. Bose National Centre for Basic Sciences, Calcutta, India — The absence of Brownian motion in granular media is a source of much complexity; among these is the presence of heterogeneity, whether static or dynamic, within a given system. Such strong heterogeneities can exist as a function of depth in a box of grains; this is the system we study here. We present results from three-dimensional, cooperative and stochastic Monte Carlo shaking simulations of spheres on heterogeneous density fluctuations. These are justaposed with results obtained from a theoretical model of a column of grains under gravity; frustrations via competing local fields is included in our model, while the effect of gravity is to slow down the dynamics of successively deeper layers. The combined conclusions suggest that the dynamics of a real granular column can be divided into different phases — ballistic, logarithmic, activated and glassy — as a function of depth. The nature of the ground states and their retrieval, in the glassy phase, shows clear evidence of intrinsic states, which lie below a band of approximately degenerate ground states. In the other three phases, by contrast, the system jams into a state chosen randomly from this upper band of metastable states.

10:00AM P8.00011 Confocal Microscopy of Shear-Induced Dynamics in Jammed Emulsions, Joaquim Clara-Rahola, Eric R. Weeks, Emory University - Physics Department — Emulsions are liquid droplets suspended in a second continuous fluid. We study polydisperse decane-in-water emulsions at droplet volume fractions of about 0.8. At such concentrations emulsions are jammed and the system exhibits the properties of a solid. Droplet rearrangements due to Brownian motion are limited in this jammed material. Thus, to induce droplet displacements at a length scale above a particle diameter, an oscillating strain is applied. We use confocal microscopy to track the trajectories of the droplets in real time and space. By taking advantage of this technique we quantify the affine and non-affine motion of the droplets due to the shear. Moreover, we study elastic and plastic droplet reconstructions as well as the spatial extent of the rearrangements when the droplet volume fraction and polydispersity are varied.

Swiss National Foundation

10:12AM P8.00012 Vacancy diffusion in a triangular lattice model, M. Jeng, M. Bowick, Syracuse University, W. Krauth, Laboratoire de Physique Statistique, Ecole Normale Superieure, J. M. Schwarz, X. Xing, Syracuse University — We study vacancy diffusion in the classical triangular lattice dimer model, subject to the kinetic constraint that dimers can only translate, but not rotate. A single vacancy—i.e. a monomer—in an otherwise fully packed lattice, is always localized in a tree-like structure. The distribution of tree sizes is asymptotically exponential and has an average of \( \langle s \rangle = 0.01 \). A connected pair of monomers has a finite probability of being delocalized. When delocalized, the diffusion is anomalous: \( \langle \tau^2 \rangle \propto t^\beta \), with \( \beta = 0.46 \pm 0.05 \). The same diffusion law is also exhibited by clusters of three or four monomers. It is found that both swap motions (translations of dimers transverse to their axes) and glide motions (translations of dimers parallel to their axes) are essential for the large-scale diffusion of monomers.

10:24AM P8.00013 Studying microscopic rearrangements in a sheared supercooled colloidal liquid, Dandan Chen, Denis Semwogerere, Joaquim Clara-Rahola, Eric R. Weeks, Emory University — Shearing induces complex microstructure changes inside an amorphous material, which is related to interesting phenomena like shear thickening and shear thinning. We use a colloidal suspension to simulate amorphous materials, and we study how shearing changes this structure using fast confocal microscopy. Many experiments and simulations have found macro-stress fluctuations in sheared dense jammed suspensions. However, the micro-rearrangements of the particles while being sheared are not very clear. We study the non-affine motion of the colloids, finding the particles move in groups, and characterize these groups for different shearing rates.

10:36AM P8.00014 Temperature control of attractive interactions in colloids, Peter Schall, University of Amsterdam, Zhbing Hu, University of North Texas — Attractive colloidal systems have attracted increasing interest recently: They exhibit phase behavior with solid, liquid, and gas phases, and various metastable states, ranging from gel-like to glassy. These colloidal systems offer a convenient way to investigate important phenomena such as phase separation and kinetic arrest. The most prominent colloidal systems are colloidal-polymer mixtures, in which the attractive strength is fixed by the concentration of the added polymer. We present a colloidal system that allows variation of the attractive potential with external control: a binary liquid solvent gives rise to temperature-dependent particle attractions close to the demixing temperature of the liquid mixture. This allows us to use temperature control to induce transitions from gas to liquid to solid, or to metastable gel-like or glassy states. Variation of the heating rate allows us to investigate the kinetics of these transitions. In this talk, I will focus on a novel system, in which close index- and density matching of the solvent and the particles is possible; this enables us to study bulk processes with temperature control.
Wednesday, March 12, 2008 8:00AM - 10:48AM –
Session P9 DFD: Microfluidic and Nanofluidic Devices
Morial Convention Center RO7

8:00AM P9.00001 Microfluidic Fabrication of Bio-compatible Vesicles by Self-assembly in Double Emulsions, HO CHEUNG SHUM, Harvard School of Engineering and Applied Sciences, Harvard University, JINWOONG KIM, Amore Pacific Co. R&D Center, DAEYEON LEE, Harvard School of Engineering and Applied Sciences, Harvard University, DAVID WEITZ, Harvard School of Engineering and Applied Sciences, and Department of Physics, Harvard University — Vesicles are compartments surrounded by bilayered membranes of amphiphilic molecules such as diblock copolymers and phospholipids. To minimize the exposure of their hydrophobic part to water, amphiphilic molecules self-assemble into aggregates of different structures. When the hydrophobic to hydrophilic ratio is close to unity, amphiphiles self assemble into bilayers, which tend to fold themselves into vesicles. These vesicles are useful for encapsulating and transporting actives such as drugs, flavor, and fragrance. To solve the problems of low encapsulation efficiency and large vesicle size distributions afforded by traditional techniques to create vesicles, we engineer a novel route to generate vesicles using monodisperse double emulsions prepared in microfluidics as templates. The double emulsion-to-vesicle transition exhibits different behaviors depending on the properties of the amphiphilic molecules such as the hydrophobic-to-hydrophilic ratio. Using this technique, we have fabricated both bio-compatible diblock copolymer vesicles, also known as polymersomes, and also lipid vesicles with high encapsulation efficiency.

8:12AM P9.00002 Glass Coating for PDMS Microfluidic Channels by Sol-Gel Methods, THAO DO, ADAM ABATE, DAVID WEITZ, Harvard University — Soft lithography in polydimethylsiloxane (PDMS) allows one to fabricate complex microfluidic devices easily and at low cost. However, PDMS swells in the presence of many organic solvents, which can significantly degrade the performance of PDMS microfluidic devices. We present a method to coat PDMS channels with a glass-like layer using sol-gel chemistry. As a demonstration of chemical resistance, we flow toluene and aqueous Rhodamine B through coated PDMS channels. Toluene is an organic solvent that significantly swells PDMS in a matter of seconds. Rhodamine B is an organic fluorescent molecule that leaches into PDMS and can therefore be used as a fluorescent probe. Indeed, the coating suppresses swelling of the channels when exposed to toluene; it also prevents leaching of Rhodamine B into PDMS channels. In addition, the channels can be functionalized with silanes to precisely control surface properties. We exploit the high chemical resistance and precise surface functionalization of the coating to produce both direct toluene-in-water and inverted water-in-toluene emulsions in coated, functionalized, PDMS microfluidic channels. This combines the ease of fabrication afforded by soft-lithography with the precision control afforded by sol-gel glass.

8:24AM P9.00003 Fluid Flow and Heat Transfer in a Dual-wet Micro Heat Pipe, JIN ZHANG, STEPHEN WATSON, HARRIS WONG, Louisiana State University — Micro heat pipes have been used to cool micro electronic devices, but their heat transfer coefficients are low compared with those of conventional heat pipes. In this talk, a dual-wet pipe is proposed as a model to study heat transfer in micro heat pipes. The dual-wet pipe has a long and narrow cavity. The bottom-half of the horizontal pipe is made of a wetting material and holds a wetting liquid, whereas the top-half is made of a non-wetting material and is filled with the vapor. As one end of the pipe is heated, the liquid evaporates and increases the vapor pressure. The higher pressure drives the vapor to the cold end where the vapor condenses and releases the latent heat. The condensate moves along the bottom half of the pipe back to the hot end to complete the cycle. Hence, the heat pipe is driven by the difference in equilibrium vapor pressure between the hot and cold ends, and not by the liquid-vapor interfacial curvature as is commonly believed. Our analysis provides an explanation for the comparatively low effective thermal conductivity in micro heat pipes [1].


8:36AM P9.00004 Measuring velocity profiles and nanoparticle interactions between 20 and 300 nm from surfaces, PATRICK TABELING, CEDRIC BOUZIGUES, ESPCI, MICROFLUIDICS TEAM — The observation of flows at a nanometric scale is crucial for understanding phenomena involving interactions between liquids and solid surfaces, such as slippage and electro-osmosis. Here we report a new method based on nanoparticle imaging by total internal reflection fluorescence, allowing the first observation of water flows between 20 and 300 nm from surfaces. We probed the energy landscape, leading to first local measurements of the Debye length and surface/nanoparticle interactions; and provide an unambiguous determination with 10 nm accuracy of the slip length for different surfaces - wetting, non-wetting, hard, soft. These results represent an improvement of one order of magnitude compared to the state of the art. In addition to investigating locally energetic and electrostatic properties of the wall/liquid system, this Letter lays down the foundations of a technique that can foster the development of nanofluidics: Imaging of Nanoparticles for Energy Landscape and Speed flow measurements (INES).

8:48AM P9.00005 Poisson-Nernst-Planck model of ion current rectification through a nanofluidic diode, DRAGOS CONSTANTIN, ZUZANNA SIWY, University of California, Irvine — We have investigated ion current rectification properties of a recently prepared bipolar nanofluidic diode. This device is based on a single conically shaped nanopore in a polymer film whose pore walls contain a sharp boundary between positively and negatively charged regions. A semiquantitative model that employs Poisson and Nernst-Planck equations predicts current-voltage curves as well as ionic concentrations and electric potential distributions in this system. We show that under certain conditions the rectification degree, defined as a ratio of currents recorded at the same voltage but opposite polarities, can reach values of over 1000 at a voltage range (-2V, +2V). The role of thickness and position of the transition zone on the ion current rectification is discussed as well. We also show that the rectification degree scales with the applied voltage.

9:00AM P9.00006 Non-reflecting boundary conditions for fluctuating hydrodynamics of compressible fluids, RAFAEL DELGADO-BUSCALIONI, Universidad Autonoma de Madrid, ANNE DEJOAN, CIEMAT, Madrid — Many important phenomena in microfluidics involve propagation of fast sound waves. Computational modeling of such problems requires a way to evacuate the reflected waves out of the computational box. However, a way to construct open boundary conditions for Fluctuating Hydrodynamics (FH) is lacking in the literature. This work presents open boundary conditions for fluctuating hydrodynamics solvers based on the Navier-Stokes Landau-Lifshitz equations. The objectives are i) ensure robust non-reflecting boundary conditions and ii) keep thermodynamic consistency for total mass fluctuation, i.e. agreement with the grand canonical ensemble. We show that by ensuring the fluctuation-dissipation balance for the total mass, one also gets the correct equilibrium power spectra of local mass and momentum at each point of the computational box. We consider real compressible fluids (argon and water) under isothermal condition and present results for the equilibrium and several out-of-equilibrium states involving generation of sound waves.

9:12AM P9.00007 ABSTRACT WITHDRAWN —
9:24AM P9.00008 Liquid precursor films spreading on chemically patterned substrates. ANTONIO CHECCO, Condensed Matter Physics and Materials Science Dept, Brookhaven National Laboratory — We study the spreading of nonvolatile liquid squalane on chemically patterned nanostrayps by using non-contact Atomic Force Microscopy (NC-AFM). The substrates are octadecyltrichlorosilane(OTS)-coated silicon wafers chemically patterned on multiple length-scales using a combination of UV and AFM oxidative lithographies. This process allows us to locally convert the terminal methyl groups of the OTS surface (non-wettable) into carboxylic acid groups (wettable) without affecting considerably the substrate roughness (<0.3nm rms). The patterned regions are shaped as a network of large (nm-sized) wettability lines connected to smaller and larger (mm-sized) lines. Liquid squalane spreads across this "microfluidic network" starting from the large lines eventually reaching the nanolines (50 to 500 nm-wide). NC-AFM is used to image the morphology of the liquid as it spreads across the nanolines. We find that the liquid thickness on the nanolines grows with time (up to ~10 nm) according to a power-law with exponent ~1. These preliminary results suggest that the spreading dynamics of laterally-confined liquids slightly differs, as expected, from the one of laterally homogeneous precursor films. We compare our findings to recent theoretical predictions of confined liquid flow and also discuss its relevance to nanofluidics.

1Supported by U.S. DOE under contract No. DE-AC02-98CH10886

9:36AM P9.00009 Velocity Dependent Selectivity of Deterministic Lateral Displacement Arrays. JASON PUCHALLA, KEITH MORTON, ROBERT AUSTIN, Princeton University — Deterministic lateral displacement (DLD) has been demonstrated as a promising microfluidic method to circumvent diffusive dispersion while separating small particles based on size. At low average flow velocity, steric repulsion and diffusion seem sufficient to describe particle behavior and array separation characteristics. However, at higher but still laminar flow velocities, particle behavior changes drastically. We have investigated this regime using a silicon DLD array. We present how the local disruption of fluid flow about a moving particle and the effects inertial forces can alter DLD behavior and can be exploited for selective sorting.

9:48AM P9.00010 Fluctuation effects and evolution in bacterial populations on a chip. JAAN MANNIK, JUAN E. KEYMER, CEEES DEKKER, Delft University of Technology — Fluctuation effects are ubiquitous in physics. Relatively little is known about what role these effects play in systems involving biological organisms. How do random fluctuations originating from the environment and from the biological organisms themselves affect the population dynamics and evolution? Here, we address this question using an experimental approach where we grow a large number of independent E. coli populations on a microfluidic silicon chip designed to evolve the body size distribution. We provide the same environmental conditions for different parental populations and follow their evolution in real time measuring number of bacteria in different colonies. We analyze fluctuations in these numbers and how the body size distribution of bacteria changes.

10:00AM P9.00011 Modelling colloidal dynamics in complex systems. CHRISTOPHER SMITH, COLIN DENNISTON, University of Western Ontario — We present a lattice Boltzmann method for dealing with solid moving boundaries in a fluid. A novel method is introduced to introduce a solid surface onto the fluid mesh. We show that for a single particle in a chute with Stokes flow, the quantitatively correct Stokes drag is obtained. Comparing two scenarios at the same Reynolds number, where the wall induces the flow or where the particle is moving, we show there is little discernible difference in the force measured. Next, we have a system with two particles and show we get quantitative agreement for the interaction between the two particles measured by our algorithm and the interaction expected according to the Rotne-Prager (RP) tensor or the Oseen tensor, in the regimes in which they are expected to be accurate. Moving away from irrotational flow, for a cylinder in a two dimensional chute the Reynolds number of the flow is increased further into the laminar region and we show the formation of eddies shedding off the solid surface. We incorporate this new algorithm into liquid crystals simulations to look at novel colloidal interactions through topological defects.

10:12AM P9.00012 Experimental and Theoretical Studies of Electroosmotic Membrane Micropumps. ZULI XU, JIA NYING MIAO, NING WANG, PING SHENG, Department of Physics and Institute of Nano Science and Technology, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China — Electroosmotic (EO) effect means fluid flow (through a porous medium) induced by an applied electric field. EO pumps have the advantages of no moving parts and easily-controlled accurate flow rate at low applied voltages. We have fabricated nano-channel EO membrane pumps using anodized aluminum oxide (AAO) as the template [1]. The diameter of the uniform-sized nanochannels can range from 60-300nm, with a membrane thickness of 30-100 microns. The EO effect is enhanced by coating the nanochannels with silica. By using de-ionized water, the nanopump performance is shown to agree reasonably well with the theoretical model, with factors such as the ratio of the double layer thickness to channel diameter, channel geometry, and treatment of the AAO membranes playing important roles. With silica coating to the nanochannels, the nanopump can produce a maximum pressure of 1 atm and a maximum flow rate of 86,000µL/min-cm2 under an applied field of 0.94 V/m. Besides DI water, the micropumps have also been tested to work well with salt, acid or base solution. [1] J.Y. Miao, Z.L. Xu, X.Y. Zhang, N. Wang, Z.Y. Yang, P. Sheng, submitted to Advanced Materials (Appeared online: 10.1002/adma.200700767).

10:24AM P9.00013 Investigation and Characterisation of Resealable Nanopores in an Elastomeric Membrane. GEOFF WILLMOTT, Industrial Research Limited — Experimental and theoretical work relating to the development of resealable synthetic nanopores will be presented. The nanopores, which are roughly conical, are formed by puncturing a relatively thick (~250 µm) elastomeric membrane with an STM tip. The aperture can be closed and the size can be dynamically controlled by stretching the elastomer [1]. Use of this technology presents a collection of interesting physical problems, covering topics that include the failure and mechanical properties of the elastomer, flow of ionic current through the aperture and particle sensing using the resistive pulse technique. Synthetic nanopores have potential applications in many fields, but especially relating to nanoscale sensing and diagnostic devices, and replication of ion channels in living cells. [1] S. J. Sowerby, M. F. Broom, G. B. Petersen, Dynamically Resealable Nanometre-Scale Apertures for Molecular Sensing, Sensors and Actuators B: Chemical 123 (1), pp. 325-330 (2007)

10:36AM P9.00014 The physics of densely-packed emulsions. DONALD M. AUBRECHT, Harvard University, DAVID F. MARRAN, DARREN R. LINK, RainDance Technologies, Inc., DAVID A. WEITZ, Harvard University — One strategy for microfluidic lab-on-a-chip applications is to use water droplets as tiny reaction vessels in a carrier stream of oil. As biochemical and cell-based experiments often require control over events that take place over a wide range of time scales, strategies need to be developed to ensure adequate timing without limiting droplet throughput. In general, longer time scales can be achieved by using longer channels or more densely packed droplets. Long channels become increasingly impractical at high throughputs for times exceeding tens of minutes, thus motivating work with densely packed droplets. Dense packing of droplets can be achieved by generating droplets on-chip, collecting them off-chip to allow the oil to drain, and re-injecting them back on-chip as a packed emulsion. This strategy is limited in that it only provides access to time scales in excess of hours. Moderate time scales can be accessed by removing carrier oil from the flow without removing the droplets. Here we present some of the physical principles governing how this can be implemented and discuss the flow of the resulting dense collections of droplets through microchannels.

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P10 DCMP: Superconducting Nanostructures | Morial Convention Center RO8
8:00AM P10.00001 Microwave Response in Short Superconducting Nanowires, ROBERT DINSMORE, MYUNG-HO BAE, ALEXEY BEZRYADIN, University of Illinois at Urbana-Champaign — Short superconducting nanowires, of length L~100 nm, have been exposed to microwave radiation (MWR) giving rise to phase slip centers that do not appear in DC measurements, without MWR. For frequencies in the 100-1000 MHz range multiple voltage jumps are observed indicating multiple phase slip centers. Each such voltage plateau is characterized by a small differential resistance, of the order of 10-20 Ohms. In this frequency range zero crossing plateaus were also observed. For frequencies from 2 to 9 GHz, MWR had a synchronization effect on the superconducting phase rotation. Resonances are observed for integer and half integer orders, similar to the original observation of Anderson and Dayem on much larger superconducting bridges [1]. [1] Anderson and Dayem, Phys. Rev. Lett. 13, p.195 (1964)

8:12AM P10.00002 Resistance in One-Dimensional Superconducting Epitaxial Niobium Nanowires, TIMOTHY MCARDLE, KEVIN INDERHEES, PAUL WELANDER, ALLISON DOVE, JAMES ECKSTEIN, Univ of Illinois Urbana-Champaign — Thermally activated phase slips cause resistance in one-dimensional superconducting wires near the critical temperature. However, this description of a thermally activated process is not able to explain additional resistance observed in extremely narrow nanowires well below Tc. We fabricate nanowires using electron beam lithography from single-crystal niobium films grown by ultra-high vacuum molecular beam epitaxy. Since the films are single crystal, the role of disorder is reduced and neither weak links nor grains are present. The films are 10 to 20 nm thick, have transition temperatures ranging from 7.2 to 9.2 K, and residual resistance ratios of 5 to 10, typical for ultra-thin single-crystal niobium films. The wires are 10 μm long and range in width from 35 to 200 nm. Transport measurements on the nanowires show two distinct regions of temperature dependence below Tc. This work was supported by the DOE BES at the F. Seitz Materials Research Laboratory at the University of Illinois, Urbana.

8:24AM P10.00003 Magnetoresistance and Critical Current Oscillations in Superconducting NbSe2 and NbN Nanowires, U. PATEL, Z.L. XIAO, J. HUA, Argonne National Laboratory and Northern Illinois University, R. DIVIAN, U. WELP, W.K. KWOK, Argonne National Laboratory — Magnetoresistances and critical currents of superconducting NbSe2 and NbN nanowires with cross-section dimensions from 300 nm to 2 μm were studied as a function of magnetic field. Sample specific oscillations were found with respect to applied magnetic field. The oscillations were completely reproducible, symmetric with respect to the direction of the field and independent of the field sweep direction. They disappeared at high fields, temperatures or currents. The oscillations were periodic in nature with superposition of more than one frequency as revealed in Fast Fourier Transform of the oscillations. The frequencies of oscillations were independent of temperature and current. Details about the transport measurements of resistance and critical current and origin of such oscillations will be discussed.

8:36AM P10.00004 “Giant” strengthening of superconducting pairing in small metallic nanoparticles: high Tc state, VLADIMIR KRESIN, Lawrence Berkeley Laboratory, YURIU OVCHENNIKOV, Landau Institute of Theoretical Physics, BAOPENG CAO, MARTIN JARROLD, Indiana University, Bloomington — The study focuses on metallic nanoclusters containing N~10^2-10^3 free carriers (e.g., Ga_{52}, Al_{25}). The delocalized cluster electrons form energy shells similar to those in atoms or nuclei. Under special conditions, superconducting pairing in such nanoclusters can become very strong, and they form a new family of high temperature superconductors. For realistic sets of parameters one can expect a high value of Tc (150 K) as well as strong modification of the energy spectrum. In principle, it is possible to raise Tc up to room temperature. Specific experiments aimed at detecting the phenomenon of pair correlation in nanoclusters can be proposed: spectroscopy, magnetic, and thermodynamic properties. Transition to the superconducting state of the cluster is accompanied by the peak in its heat capacity. The phenomenon is promising for the creation of high Tc superconducting tunneling networks, and hence macroscopic superconductivity.

8:48AM P10.00005 Evidence for High Tc Superconducting Transitions in Isolated Al_{45} and Al_{47} Nanoclusters, MARTIN JARROLD, BAOPENG CAO, COLLEEN NEAL, ANNE STARACE, Indiana University, YURIU OVCHENNIKOV, Landau Institute for Theoretical Physics, VLADIMIR KRESIN, Lawrence Berkeley Laboratory — Heat capacities measured for Al_{45} and Al_{47} nanoclusters have reproducible peaks at ~ 200 K. The data were obtained using a multi-collision dissociation method [1] allowing us to perform measurements for isolated nanoclusters. The peaks are observed for selected Al clusters only. These peaks are consistent with theoretical predictions that some clusters with highly degenerate electronic states near the Fermi level will undergo a transition into a high Tc superconducting state [2]. An analysis based on a theoretical treatment of pairing in Al_{45} and Al_{47} agrees well with the experimental data in both the value of the critical temperature and in the size and width of the peaks in the heat capacity. The observed value of Tc exceeds those found in bulk systems. [1] G.Breaux, C.Neal, B.Cao, M.Jarrod, Phys. Rev. Lett. 94, 173401 (2005) [2] V.Z.Kresin, Yu.Ovcchinnikov, Phys. Rev. B 74, 024514 (2006)

9:00AM P10.00006 Quantum confinement effects on superconducting properties of Lead nanocrystals, HERVE AUBIN, CNRS-ESPCI, HELENA MOREIRA, UPM6, BENOIT MAHLER, ESPCI, BENOIT DUBERTRET, CNRS-ESPCI — We developed a new chemical synthesis method for producing large quantities of monodispersed lead (Pb) nanocrystals. They are obtained from the alcohol reduction of a mixture of two lead carboxylates with alkyl chains of different lengths, dissolved in a high temperature solvent. The nanocrystals obtained are monodispersed particules are obtained when nucleation and growth occur at distincts temperatures, possibly as a consequence of different reactivities of the reagents. The delocalized cluster electrons form energy shells similar to those in atoms or nuclei. Under special conditions, superconducting pairing in such nanoclusters can become very strong, and they form a new family of high temperature superconductors. For realistic sets of parameters one can expect a high value of Tc (150 K) as well as strong modification of the energy spectrum. In principle, it is possible to raise Tc up to room temperature. Specific experiments aimed at detecting the phenomenon of pair correlation in nanoclusters can be proposed: spectroscopy, magnetic, and thermodynamic properties. Transition to the superconducting state of the cluster is accompanied by the peak in its heat capacity. The phenomenon is promising for the creation of high Tc superconducting tunneling networks, and hence macroscopic superconductivity.

9:12AM P10.00007 Superconductivity of nano-size Pb Islands studied by low-temperature scanning tunneling microscopy / spectroscopy, TAKAHIRO NISHIO, TOSHU ATSUMI, ANTSUHI NOMURA, KOUSUKE MIYACHI, TOYOAKI EGUCHI, YUKIO HASEGAWA, Inst. Solid State Phys., Univ. Tokyo, HIDEAKI SAKATA, Tokyo Univ. of Science — Nano-size superconducting materials, whose dimensions are comparable with or smaller than their coherent length / penetration depth, behave differently from bulk superconductors. By forming structures using lithographic methods various unique properties of mesoscopic superconductors have been elucidated. Since these studies, however, measure electrical conductance and / or magnetization, details inside the superconductors cannot be directly probed. In this study we investigated superconductivity inside superconductors by directly measuring the superconducting gaps over ultra thin Pb island structures using a LT-STM at 2.0 K [1]. The obtained tunneling spectra exhibit an increment of zero bias conductance (ZBC) with a magnetic field and its dependence on the lateral size of the islands. Moreover, from spatial mappings of ZBC, the island size dependence and spatial variation of superconductivity inside of each island are visualized. We found that the number of vortices piercing the islands before breakdown of superconductivity depends on the lateral size of the islands. Details of the size-dependent critical fields are discussed at the presentation. [1] Nishio et al., APL 88, 113115 ’06, JAP 46, L880 ’07.
9:24AM P10.00008 Flux jump in superconducting Pb networks at fractional numbers of the matching fields, TAKEKAZU ISHIDA, YOSHIKAZU MATSUSHIMA, MAKOTO SHIMIZU, Osaka Prefecture University, MASAHIKO HAYASHI, Akita University, HIROMICHI EBISAWA, Tohoku University, MASARU KATO, Osaka Prefecture University, OSAMU SATO, Osaka Prefectural College of Technology, NEYAGAWA, KAZUO SATO, TSUTOMU YOTSUYA, Technology Research Institute of Osaka Prefecture — The extended Little-Parks effect of superconducting network is known as a periodic Tc variation as a function of magnetic field. Superconducting Pb honeycomb networks of matching field 0.106 G and triangular microhole lattice of Pb of matching field 0.425 G have been fabricated by the combined techniques of the electron beam lithography and a lift-off process of evaporated Pb films. The application of magnetic field corresponds to the vortex doping into networks. We measured the magnetization of the networks systematically by using a SQUID magnetometer. We found that flux jump appears rather periodically as a function of magnetic field. Flux jumps may be induced by a periodic decrease in the critical current density of the network. To the authors’ knowledge, this is for the first time to observe the extended Little-Parks effect appeared in flux jumps. We also discuss the anomalous matching effect.

9:36AM P10.00009 Switching Current Distributions of Superconducting Nanowires: Evidence for Individual Quantum Phase Slips, MITRABHANU SAHU, MYUNG-HO BAE, UIUC, ANDREY ROGACHEV, University of Utah, DAVID PEKKER, Harvard University, NAYANA SHAH, UIUC, TZU-CHIEH WEI, University of Waterloo, PAUL GOLDBART, ALEXEY BEZRYADIN, UIUC — Phase slip fluctuations cause premature stochastic switching of the state of a current biased quasi-one-dimensional nanowire from superconducting to normal at sub-critical currents. Here, we report on measurement of the distributions of switching currents performed on amorphous superconducting MoGe/Co21 nanowires over a range of temperatures. The measured widths of the switching current distributions are observed to increase with decreasing temperature. We explain this counterintuitive result by considering a microscopic stochastic model of heating caused by each phase slip event. The measured rates of escape from the superconducting state agree well with the predictions of the stochastic model under the assumption of phase slippage by thermal activation at relatively high temperatures and macroscopic quantum tunneling at sufficiently low temperatures. We identify and explore a region in which a single quantum phase slip is all that is necessary to trigger switching from the superconducting to the normal state.

9:48AM P10.00010 Theory of superconductive-resistive switching in nanowires due to heating by stochastic phase slips, NAYANA SHAH, University of Illinois at Urbana-Champaign, DAVID PEKKER, Harvard University, PAUL GOLDBART, University of Illinois at Urbana-Champaign — We study the stochastic dynamics of superconductive-to-resistive switching in hysteretic current-biased superconducting nanowires undergoing phase-slip fluctuations. We assume that the hysteresis is thermal in nature, and postulate that the mechanism for the switching is thermal runaway, i.e. random sequences of stochastic phase slips, closely spaced in time, that heat the nanowire. Thus, via the master-equation formalism, we obtain the distribution of currents at which switching occurs. If switching were caused by single, thermally-activated phase-slip events then this distribution would narrow as the temperature is reduced. However, at higher temperatures we find that several phase-slip events are typically necessary for inducing switching, and this results in an initial broadening of the distribution upon cooling. Quite generally, we predict that at low temperatures thermal runaway is caused by a single phase-slip event. Thus, measurements of switching-current distributions in this regime are a direct probe of this basic collective process. In particular, this regime could yield observations of individual quantum phase slips in nanowires.

10:00AM P10.00011 Anisotropic Superconductivity in MoGe - Permalloy Bilayers1, GORAN KARAPETROV, Argonne National Lab, A. BELKIN, ANL and Illinois Institute of Technology, V. NOVOSAD, M. IAVARONE, J. FEDOR, Argonne National Lab, A. TRONCALLI, Austin College, J. PEARSON, W.K. KWOK, Argonne National Lab — We studied the magnetico-transport properties of superconductor-ferromagnet MoGe/Permalloy bilayers. The ferromagnet with stripe domain structure induces in-plane anisotropy in superconducting order parameter. Superconducting phase diagram shows that near the S-N phase boundary the superconductivity is localized in narrow mesoscopic channels just above the magnetic domain walls. We determined the scaling phase diagram, which shows that even in wider samples the PSS contribution dominates over vortices in a substantial region of current/temperature variations [1]. The above fluctuations generated by topological excitations also provide a noise limit to superconducting detectors operating in a resistive state, e.g. for dark counts in single-photon detectors. [1] M. Bell et al., Phys. Rev. B 76, 094521 (2007).

1This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357.

10:12AM P10.00012 Superconductor-Ferromagnet Bilayers: Influence of Magnetic Domain Structure on Vortex Dynamics1, ANDREY BELKIN, Argonne National Laboratory and Illinois Institute of Technology, V. NOVOSAD, M. IAVARONE, J. PEARSON, W.K. KWOK, G. KARAPETROV, Argonne National Laboratory — We investigate the influence of orientation of stripe-like domain structure in ferromagnetic films on vortex dynamics in superconductor-ferromagnet bilayers. We measure transport properties in different external magnetic fields applied perpendicular to the surface of the bilayers. Parameters of superconductor-ferromagnet bilayers are such that domain period is much bigger than the superconducting coherence length but much smaller than the effective penetration depth. Prominent dissimilarity of critical currents of two studied bilayers runs systematically by using a SQUID magnetometer. We found that flux jump appears rather periodically as a function of magnetic field. Flux jumps may be induced by a periodic decrease in the critical current density of the network. To the authors’ knowledge, this is for the first time to observe the extended Little-Parks effect appeared in flux jumps. We also discuss the anomalous matching effect.

1This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357.

10:24AM P10.00013 Topological excitations in superconducting nanostripes: Resistive States and Noise1, MATT BELL, ANDREI SERGEEY, VLADIMIR MITIN, ALEKSANDR VEREVKIN, SUNY at Buffalo — We investigate competition between one- and two-dimensional topological excitations - phase slips and vortices - in formation of resistive states and noise generation in ultrathin superconducting Bi2122Nanostripes in a wide temperature range below the mean-field transition temperature Tc0. The widths w = 100 nm of our ultrathin Bi2122 nanostructures are substantially larger than the Ginzburg-Landau coherence length ξ = 4nm and the fluctuation resistivity above Tc0 has a two-dimensional character. However, our data shows that the resistivity below Tc0 is produced by one-dimensional excitations, - thermally activated phase slip strips (PSSs) overlapping the sample cross-section. We determine the scaling phase diagram, which shows that even in wider samples the PSS contribution dominates over vortices in a substantial region of current/temperature variations [1]. The above fluctuations generated by topological excitations also provide a noise limit to superconducting detectors operating in a resistive state, e.g. for dark counts in single-photon detectors. [1] M. Bell et al., Phys. Rev. B 76, 094521 (2007).

1This work was supported by NYSTAR grant and NSF IGERT program.
10:36AM P10.00014 Nonlinearities and Parametric Amplification of Superconducting Coplanar Waveguide Resonators1, DAVID HAVILAND, ERIK THOLÉN, ADEM ERGUL, Royal Institute of Technology KTH, NANOSTRUCTURE PHYSICS KTH TEAM — We have experimentally studied the nonlinear properties of superconducting coplanar stripline resonators fabricated from Al and Nb films with small transverse dimensions (gap size 1 µm). Magnetic field penetration into the superconductor causes a current-dependant kinetic inductance, which gives an ideal Kerr nonlinearity. When the nonlinear oscillator is pumped very near its dynamic instability, it can be used to realize parametric amplification. We have achieved a gain of ~22.4 dB in a 5.8 GHz resonator cooled to 450 mK [E. Tholén et. al. Appl. Phys. Lett. 90, 253509 (2007)]. Parametric deamplification or squeezing of a signal has also been verified with squeezing of 30 dB. The later effect is interesting because it can be used to generate squeezed vacuum states of the electromagnetic field. We have modeled the data using a theory developed by Yurke and Buks [I. Lightwave Technol. 24, 6054 (2006)]. Excellent fit of the model to the measured data can be achieved over a wide range of pump power, and the strength of the nonlinear terms can be obtained with high accuracy.

1Work Supported by the Swedish VR.

10:48AM P10.00015 Observation of Nonlocal Coherence Between Normal Metals Coupled by a Superconductor1, PAUL CADDEN-ZIMANSKY, JIAN WEI, VENKAT CHANDRASEKHAR, Northwestern University — In conventional superconductors the effective size of the constituent Cooper pairs can approach several hundred nanometers, a length scale accessible by nanolithographic techniques. By placing two normal metals on a superconductor within a coherence length of each other, it has been predicted that the quasiparticles in the separate metals can be coherently coupled by the Cooper pairs through the nonlocal processes of Elastic Cotunneling and Crossed Andreev Reflection. We present experimental observations of coherent, nonlocal thermoelectric effects between normal metals coupled to a superconductor by using a hybrid normal-superconductor interferometer. The sign of the observed thermoelectric voltage can be switched using an external field, indicating that the voltage is dynamically driven by a persistent current induced in the interferometer.

1Supported by NSF Grant No. DMR-06-04601

Wednesday, March 12, 2008 8:00AM - 10:24AM —
Session P11 DMP: Focus Session: MgB2-like: Disorder in Novel Superconductors Morial Convention Center R09

8:00AM P11.00001 Penetration depth study of Li, C and Li+C doped MgB2 single crystals, CATALIN MARTIN, MATTHEW VANNETTE, RUSLAN PROZOROV, Ames Laboratory, Ames, IA 50011, J. KARPINSKI, N. ZHIKADLO, R. KHASANOV, Laboratory for Solid State Physics, ETH, 8093 Zurich, Switzerland — Magnetic penetration depth was studied in single crystals of MgB2, pure and doped with Li, C and Li+C. At zero applied field London penetration depth is measured and superfluid density, n_s, can be evaluated. We analyze effect of the dopings on n_s, thus on the superconducting gaps. In the vortex state, Campbell penetration depth is measured and it provides information about true critical current unaffected by the magnetic relaxation. In particular, penetration depth in vortex state becomes strongly irreversible, and we show that C doping enhances the irreversibility region, whereas the substitution with Li does not affect the results. They are discussed in terms of two-gap nature of MgB2.

1Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

8:12AM P11.00002 Nano-scale TiB2 Precipitates in MgB2 Superconducting Wire1, D.K. FINNEMORE, M.E. TILLMAN, P.C. CANFIELD, S.L. BUD’KO, Y.Q. WU, M.J. KRAMER , Ames Lab / Iowa State University, J.V. MARZIK, Specialty Materials, Inc., Lowell, MA, M. RINDFLEISCH , Hyper Tech Research Inc., Columbus, OH , S.T. HANNAHS, NHMFL, Tallahassee, FL — Superconducting MgB2 wire containing uniformly dispersed, nano-scale TiB2 precipitates has been produced using a plasma synthesis method to make the starting Ti doped B powder. A powder-in-tube method is used for making the wire. Sub-micrometer size MgB2 grains are decorated with a random dispersal of 5 to 20 nm precipitates. The superconducting properties are reported for a family of powder-in-tube wires fabricated with pure boron, carbon doped boron, and titanium doped boron. The particle size of the doped boron powder, of 50 to 100 nm, permits low reaction temperatures and short reaction times. The sign of the observed thermoelectric voltage can be switched using an external field, indicating that the voltage is dynamically driven by a persistent current induced in the interferometer.

8:24AM P11.00003 Properties of Carbon Doped MgB2 Films by HPCVD Using TMB, WENQING DAI, R.H.T. WILKE, KE CHEN, QI LI, XIAOXING XI1, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania, USA — Carbon-doping is an effective way to enhance the upper critical field of MgB2. Our previous carbon-alloyed MgB2 films using (MeCp)2Mg as the carbon source show dramatically increased Hc2 values to over 60 T at low temperatures. Structure analyses of these films indicate that only part of the carbon is doped into the MgB2 lattice and the rest forms highly resistive foreign phases in the grain boundaries. To fabricate more homogeneously carbon doped thin films, gaseous trimethylboron (TMB) was used as the carbon source. The normal state resistivity of carbon doped films using TMB increases much more slowly with carbon concentration, demonstrating a better connection between the MgB2 grains. However the relatively high growth temperature, required to decompose TMB, limits the film thickness in the original Hybrid Physical-Chemical Vapor Deposition (HPCVD) setup. A hot wire is then installed in the HPCVD system to help decompose TMB while the substrate and Mg bulk source are kept at relatively low temperature. Initial results of these films will be presented.

1Also with Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA

8:36AM P11.00004 Inhomogeneous Nanoscale Disorder in Doped Magnesium Diboride1, PAUL VOYLES, University of Wisconsin, Madison — Using TEM and STEM imaging and microanalysis, we have shown that doped MgB2 has a variety of forms of disorder at a length scale of 5-50 nm. In [0001]-normal, carbon-doped HPCVD thin films, there is a thin, amorphous, C-rich layer which separates domains of lightly carbon-doped MgB2. Carbon also causes significant spread in the local in-plane orientation and c-axis direction of the MgB2. We also observed disorder in the orientation of small MgB2 domains in oxygen-doped thin films grown by MBE. Both of types of films show dramatic enhancement in the upper critical magnetic field compared to pure MgB2, with extrapolated Hc2(0 K) reaching 65-70 T for some samples. The origin of this increase may be in the observed disorder, particularly in confinement of the superconducting MgB2 domains by non-superconducting second phase layers.

1This work was supported by the NSF FRG on Magnesium Diboride, DMR-0514592.
9:12AM P11.00005 The Ca and Yb Isotope Effect in Superconducting Ca and YbC12

DAVID HINKS, DAN ROSENMANN, HELMUT CLAUS, Argonne National Laboratory — The isotope effect \((\alpha = -\log T_c/\log M)\) where \(M\) is the isotope mass and \(T_c\) is the transition temperature \((300 \text{K})\) is a measure of the phonon contribution to the superconductivity. We have measured both the Ca and the Yb isotope effect in intercalated highly orientated pyrolytic graphic (HOPG) by vapor phase transport of the isotopes. We find a large and, within the experimental error, equal \(\alpha\) for each element, \(0.36(4)\) and \(0.40(4)\) for Yb and Ca, respectively. The value for Ca is larger then theoretically predicted indicating a stronger electron-phonon coupling.

3Work supported by DOE Office of Science under Contract No. DE-AC02-06CH11357.

9:24AM P11.00006 Crystal Structures and Physical Properties of One-Dimensional Borides

A11+MFe4B12 \((A = \text{Ca, Y; La; } M = \text{Fe, Co, Ru})\), YUKARI KATSURA, HIRAKU OGINO, YUTAKA MATSUMURA, SHIGERU HORII, JUN-ICHI SHIMOYAMA, KOHIJI KISHIO, Dept. of Applied Chemistry, Univ. of Tokyo — We investigated crystal structures and physical properties of La11+Fe4B12 (\(\varepsilon \approx 0.06\)) and three new borides Y11+Fe4B12 (\(\varepsilon \approx 0.16\)), CaCo4B12 and Ca11+Ru4B12 (\(\varepsilon \approx 0.13\)). Poly crystalline bulk samples were obtained by reacting metal boride precursors (FeB, CoB, RuB) with La, Y and La metals. Microstructure were analyzed using a SEM with an EDX. Crystal structures were analyzed through XRD and Rietveld analysis of powder XRD patterns. Electrical resistivity and magnetization measurements were carried out from 1.8 to 300 K. We found that all these compounds belong to the same structural family as RE11+Fe4B12 (RE = La-Tm): a tetragonal lattice composed of one-dimensional channels of FeB and single atomic chains of RE. Incommensurate structures along c-axis were observed in La11+Fe4B12, Y11+Fe4B12 and Ca11+Ru4B12. The La11+Fe4B12 bulks exhibited type-II superconductivity below 6.0 K, although this might be due to the superconductivity of dirty \(\beta\)-La remaining in the bulks. The other new borides did not show superconductivity down to 1.8 K.

9:36AM P11.00007 Observation of a new phase in the Li-B system.

EDUARD GALSTYAN, YUYI XUE, YANYI SUN, IRENE RUSAKOVA, TsSUH and Department of Physics, University of Houston, NING WANG, Department of Physics, The Hong Kong University of Science and Technology, KAREN MKHOYAN, Department of Applied and Engineering Physics, Cornell University, CHING-WU CHU, TsSUH, The Hong Kong University of Science and Technology, Lawrence Berkeley National Laboratory — The simple compounds of boron and light elements have attracted interest since the unexpected discovery of high temperature phonon-coupled superconductivity (SC) in MgB2. The numerous theoretical works show that the Li-B system has electronic features similar to those in MgB2 and compounds in the system are expected to be superconducting. In fact, there were early reports of Li-B compounds. Although the small Li-size suggests a rich phase diagram, the previous investigations discovered only one stable compound over a broad initial stoichiometry. The extreme reactivity and hydrolyses of Li in air may be partially responsible for this. We were able to synthesize a new Li-B pure phase that belongs to hexagonal symmetry through a new synthesis procedure. We report on the structural, magnetic, and electron energy loss spectra (EELS) analyses of this compound. Despite the similarity with the electronic structure of MgB2, the Li-B system has not yet shown the existence of SC.

9:48AM P11.00008 Superconductivity in heavily boron-doped single crystalline and nanocrystalline diamond thin films

P. ACHATZ, C. MARCENAT, CEA Grenoble/DRFMC/SPSMS, France, E. BUSTARRET, T. KLEIN, CNRS Grenoble/Institut Niel, France, O.A. WILLIAMS, Institut for Materials Research, Belgium, J.A. GARRIDO, M. STUTZMANN, WSI TUM, Germany — Our results show that the critical boron concentration \(n_B\) for single crystalline diamond (scd) and nanocrystalline diamond (ncd) thin films is the same for the normal to superconducting and for the non-metal to metal transitions, on the order of 5 \times 10^{20} \text{ cm}^{-3}, in agreement with estimates derived from various theoretical approaches. In scd material, a variable range hopping behaviour was clearly observed on the insulating side of the transition, and, as expected, the characteristic temperature \(T_H\) tended toward zero at the transition. On the metallic side, the zero temperature conductivity \(\sigma_0\) scaled with \((n_B/n_c \sim 1)^{\nu} \approx 1\). The critical temperature \(T_c\) remained high in the vicinity of the metal-non metal transition, and it was rather found to scale with \((n_B/n_c \sim 1)^{3/2}\). These results led us to propose that the electron-phonon coupling parameter \(\lambda\) remains large down to \(n_B/n_c \approx 1\), and to examine the metal-insulator transition and the parameter set \((\lambda, \mu)\) in terms of scaling laws.

Low temperature magnetotransport measurements and the possible occurrence of a superconductor-insulator transition in heavily boron-doped ncd will be discussed.

10:00AM P11.00009 Tracing the evolution of two energy gaps of MgB2 with increasing disorder

MAURICIO ESCOBAR M., YONG-JIHN KIM, University of Puerto Rico — Previously we have determined the phonon-mediated matrix elements for MgB2 using the two band model and the scattered states. We noticed that, in the dirty limit, where the resistance ratio is about 3, the impurity scattering does not reduce the matrix elements much due to the Cooper pair size effect, whereas, in the weak localization limit, where the resistance ratio is less than 3, all the matrix elements are decreasing significantly due to weak localization. Now we calculate numerically the matrix elements and solve the gap equations with increasing disorder. We determine when the two energy gaps merge into one common energy gap and compare our calculations with experiments. We also calculate the transition temperature, \(T_c\), as a function of the resistance ratio.

10:12AM P11.00010 Magnetic field-tuned superconductor-insulator transition in quenched-condensed ultrathin Be films

ZUXIN YE, WENHAO WU, Texas A & M University — We quenched condensed ultrathin Be films onto glass slides inside a dilution refrigerator with the substrates held near 10 K. The films were first tuned from insulating to superconducting by increasing the thickness in fine steps. The thickness-tuned transition occurs at a normal state sheet resistance \(R_N \sim 13 \text{ k-Ohm measured at } 10 \text{ K.}\) For superconducting films of various thickness, the field-tuned superconductor-insulator transition was then investigated. Remarkably, the critical resistance of the field-tuned transition was found to be \(R_C = \sim 4/6\), independent of the thickness of films of \(R_N\) ranging from 11 to 6 k-Ohm, critical temperature \(T_c\) ranging from 1.3 to 5.2 K, and critical field \(B_C\) ranging from 1 to 8 T. This result is a strong evidence for a duality quantum phase transition from a vortex glass in the superconducting state to a Bose glass in the field-induced insulating state. For thicker films with \(R_N < 5 \text{ k-Ohm, the critical resistance no longer remained at } h/4e^2\) but was nearly equal to \(R_N\). This observation suggested that these thick films were no longer in the vicinity of the quantum critical point.

1This work is supported by NSF under Grant Nos. DMR-0551813 and DMR-0606529.

Wednesday, March 12, 2008 8:00AM - 10:48AM –
Session P12 GFC: Skutterudites and Other Heavy Fermions Morial Convention Center 203

8:00AM P12.00001 Metal-insulator and metal-metal behavior in filled-skutterudites

LING YANG, SHAN-WEN TSAI, Department of Physics & Astronomy, UC Riverside — Filled-skutterudites compounds are of the form \(LT_{2.1}X_{12}\), where \(L\) stands for Lanthanide, \(T\) stands for transition metal and \(X\) stands for Pnictogen. They show many unusual properties, and are also important due to their thermo electric properties. Here we focus on the metal-insulator and metal-metal behavior observed in \(PrRu_2P_{12}\) and \(PrOs_2P_{12}\) compounds. We propose a simple model where the positions of the L atoms in different minima inside the cage, and a phase transition occurs when the temperature is lowered. The nature of the transition depends on the density of carriers.
Andreev spectroscopy study of multigap pairing in PrOs$_4$Sb$_{12}$. C.S. Turel, J.Y.T. Wei, University of Toronto, B. Djurkovic, J.B. Kycia, University of Waterloo, W.M. Yuhasz, R. Baumbach, M.B. Maple, University of California at San Diego — The recent discovery of superconductivity in the filled skutterudite heavy fermion material PrOs$_4$Sb$_{12}$ has generated widespread interest. Different experimental studies have reported various field- vs-temperature phase diagrams, with mixed evidence for nodes in the pairing gap. Some experiments have also indicated the presence of multiple gaps, suggesting that the pairing involves multiple bands or multiple order parameters. We present Andreev spectroscopy data, down to 80 mK and up to 2.5 T, taken using ballistic point contacts made with Pt-Ir tips on single crystals of Pr(Os$_{1-y}$Ru$_y$)$_4$Sb$_{12}$. We observed distinct spectral evidence for gap nodes. We also observed multiple spectral features arising from Ru-doping. We interpret the evolution of these spectral features within the scenario of multigap pairing.


Defects and broken time-reversal symmetry in superconducting Pr(Os$_4$Ru$_4$)$_4$Sb$_{12}$. D.E. MacLaughlin, LEI SHU, U. Calif., Riverside, A.D. Hillier, ISIS, Rutherford Appleton Lab., O.O. Bernal, Calif. State U., Los Angeles, Y. Aoki, D. Kikuchi, H. Sato, Y. TunaShima, T.A. Sayles, T. Yanagisawa, W.M. Yuhasz, M.B. Maple, U. Calif., San Diego — Muon spin relaxation studies of a spontaneous local field $H_L$ in a powder sample of PrOs$_4$Sb$_{12}$, previously observed in the superconducting state of PrOs$_4$Sb$_{12}$ and attributed to broken time-reversal symmetry, have been extended to PrRu$_4$Sb$_{12}$ and PrOs$_4$Ru$_4$Sb$_{12}$ by means of quasielastic muon spin relaxation with $H_L > 0.1 T$. The effect is reduced by a factor of 2 in PrRu$_4$Sb$_{12}$, and in PrOs$_4$Ru$_4$Sb$_{12}$ it is strongly suppressed but remains observable for $x \leq 0.2$. In powder samples prepared by solid state reaction, however, no field is observed for $x = 0.1$ or 0.2. Muon spin relaxation due to dynamic $^{141}$Pr nuclear spin fluctuations is reduced in the powders. Both results can be understood if the density of microscopic defects is smaller in the powders: defects increase muon spin relaxation by $^{141}$Pr spins, and supercurrents associated with defects are predicted to create spontaneous fields in TRS-breaking superconductors. Our results are strong experimental evidence for this prediction.

Multi-symmetry and Multi-band Superconductivity in Superconducting Filled-skutterudites. R.W. Hill, University of Waterloo, Canada, S.H. Li, Universite de Sherbrooke, Canada, M.B. Maple, University of California, San Diego, L. Taillefer, Universite de Sherbrooke, Canada — Thermal conductivity measurements were performed on single crystal samples of the superconducting filled skutterudite compounds PrOs$_4$Sb$_{12}$ and PrRu$_4$Sb$_{12}$ both as a function of temperature and magnetic field applied perpendicular to the heat current. In zero magnetic field, the low temperature electronic thermal conductivity of PrRu$_4$Sb$_{12}$ vanishes at low temperatures, consistent with a fully-gapped Fermi surface. For PrOs$_4$Sb$_{12}$, however, we do not find clear evidence for residual electronic conduction as the temperature tends to zero Kelvin which is consistent with the presence of nodes in the superconducting energy gap. The field dependence of the electronic conductivity for both compounds shows a rapid rise immediately above $H_T$, and a significant structure over the entire vortex state. For both compounds, superconducting properties imply a $d$-wave state and significant structure over the entire vortex state. In the fully gapped superconductor PrRu$_4$Sb$_{12}$, this is interpreted in terms of multi-band effects. In PrOs$_4$Sb$_{12}$, we consider the Doppler shift of nodal quasiparticles at low fields and multiband effects at higher fields.

High-field de Haas-van Alphen investigation of the filled skutterudite compound NdOs$_4$Sb$_{12}$. P.-C. Ho, Physics/CSU-Fresno, J. Singleton, NHML/LANL, M.B. Maple, Physics/UCSD, P. Goddard, Physics/Oxford U., T. Yanagisawa, Nagita U., Japan — The filled skutterudite compound NdOs$_4$Sb$_{12}$ displays mean-field type ferromagnetism with a Curie temperature of $0.9\text{K}$. The spontaneous magnetization of this compound is $0.75\text{K}$ at $T = 0$. The magnetization is strongly suppressed but remains observable for $x \leq 0.2$. In powder samples prepared by solid state reaction, however, no field is observed for $x = 0.1$ or 0.2. Muon spin relaxation due to dynamic $^{141}$Pr nuclear spin fluctuations is reduced in the powders. Both results can be understood if the density of microscopic defects is smaller in the powders: defects increase muon spin relaxation by $^{141}$Pr spins, and supercurrents associated with defects are predicted to create spontaneous fields in TRS-breaking superconductors. Our results are strong experimental evidence for this prediction.

Non-Fermi liquid behavior in the filled skutterudite compound CeRu$_4$As$_{12}$. R. Baumbach, Physics and IPAPS, UCSD, P.-C. Ho, CSU Fresno, T. Sayles, M.B. Maple, Physics and IPAPS, UCSD, R. Vawreyk, T. Cichorek, A. Pietraszko, Z. Henkie, Low T and Struct, Polish Acad. of Sci. — The filled skutterudite compounds of the form MT$_2$X$_{12}$ (M = alkali metal, alkaline earth, lanthanide, actinide, T = Fe, Ru, Os and X = P, As, Sb) exhibit a wealth of strongly correlated electron phenomena. The CeT$_2$X$_{12}$ subclass is interesting since it includes the only filled skutterudite known to show non-Fermi liquid (NFL) behavior. CeRu$_4$As$_{12}$, in addition to various semiconductors where the gap-size is controlled by the lattice constant. We present electronic resistivity, specific heat, and magnetic susceptibility measurements for the new compound, CeRu$_4$As$_{12}$, which reveals NFL T-dependences at low T, i.e., $\rho(T) \sim T^{1-\delta}$ and weak power law or logarithmic divergences in $C(T)/T$ and $\chi(T)$. Measurements also show that the T-dependence of the thermoelectric power $S(T)$ deviates from that in other Ce systems. The NFL behavior appears to be associated with a nonmagnetic or weakly magnetic ground state, as revealed by magnetization M(H,T) measurements.

Non-Fermi liquid behavior in the filled skutterudite compound CeRu$_4$As$_{12}$. R. Baumbach, Physics and IPAPS, UCSD, P.-C. Ho, CSU Fresno, T. Sayles, M.B. Maple, Physics and IPAPS, UCSD, R. Vawreyk, T. Cichorek, A. Pietraszko, Z. Henkie, Low T and Struct, Polish Acad. of Sci. — The filled skutterudite compounds of the form MT$_2$X$_{12}$ (M = alkali metal, alkaline earth, lanthanide, actinide, T = Fe, Ru, Os and X = P, As, Sb) exhibit a wealth of strongly correlated electron phenomena. The CeT$_2$X$_{12}$ subclass is interesting since it includes the only filled skutterudite known to show non-Fermi liquid (NFL) behavior. CeRu$_4$As$_{12}$, in addition to various semiconductors where the gap-size is controlled by the lattice constant. We present electronic resistivity, specific heat, and magnetic susceptibility measurements for the new compound, CeRu$_4$As$_{12}$, which reveals NFL T-dependences at low T, i.e., $\rho(T) \sim T^{1-\delta}$ and weak power law or logarithmic divergences in $C(T)/T$ and $\chi(T)$. Measurements also show that the T-dependence of the thermoelectric power $S(T)$ deviates from that in other Ce systems. The NFL behavior appears to be associated with a nonmagnetic or weakly magnetic ground state, as revealed by magnetization M(H,T) measurements.

Low-temperature thermal and transport properties of single-crystalline Ce$_4$Pt$_2$Sn$_{25}$. Nobuyuki Kurita, Han-Oh Lee, Yoshifumi Tokiwa, Eric Bauer, Joe Thompson, Los Alamos National Laboratory, Zachary Fisk, Department of Physics, University of California Davis, PEI-Chun Ho, M. Brian Maple, Department of Physics and Institute for Pure and Applied Physical Sciences, University of California-San Diego, Roman Movshovich, Los Alamos National Laboratory — Low-temperature specific heat $C(T)$ and electrical resistivity $\rho(T)$ measurements have been performed on a flux-grown single-crystalline Ce$_4$Pt$_2$Sn$_{25}$ which has a body-centered cubic structure. As temperature decreased, $C(T)$ increased and showed a huge jump $(\Delta C/T \sim 43 J/mole-K^2-Ce)$ at $T \sim 0.2 K$, probably due to a magnetic ordering. The entropy gain connected with the ordering reaches a half of $C(T)$ at $T = 0.2 K$. Corresponding to the degeneracy of the fundamental crystal-field doublet. On the other hand, $\rho(T)$ showed metallic behavior and decreased rapidly around the ordering temperature with a clear kink. We will also discuss the results of external-field effect on this compound.

Acknowledgements: This work was supported by NSERC, CF1/IOIT, Canadian Institute for Advanced Research and U. S. Department of Energy Grant No. DE-FG02-04ER46105.
9:24AM P12.00008 Magnetodynamics of Heavy Fermion YbCo$_2$Zn$_{20}$ and YbFe$_2$Zn$_{20}$, A.D. CHRISTIANSON, Oak Ridge National Laboratory, Oak Ridge 37831, TN USA, E.A. GOREMYCHKIN, Argonne National Laboratory, Argonne, IL 60439, USA, MICHAEL M. KOZÁ, Institut Laue-Langevin, FR-38042 Grenoble, France, J.L. ZARESTKY, Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA, C.H. WANG, University of California, Irvine, California 92697, USA, A.I. KOLESNIKOV, Argonne National Laboratory, Argonne, IL 60439, USA, N. NI, S. JIA, E.D. MUN, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory and Department of Physics, Iowa State University, Ames, Iowa 50011, USA — We have performed inelastic neutron scattering experiments on the recently discovered heavy Fermion systems YbCo$_2$Zn$_{20}$ and YbFe$_2$Zn$_{20}$. The magnetic excitation spectrum demonstrates that YbCo$_2$Zn$_{20}$ exhibits crystal field dynamics with an overall splitting of 2.72 meV. Despite this, the splitting between the ground state and first excited state is large enough such that the large low temperature electronic specific heat is not due to crystal field entropy and hence YbCo$_2$Zn$_{20}$ is a truly heavy Fermion material. YbFe$_2$Zn$_{20}$ exhibits significantly different spin dynamics. At 200 K the scattering is quasilastic and as the temperature is lowered the spectral weight is progressively shifted to finite energy transfers. This temperature dependence is characteristic of an intermediate valence system with an unusually low Kondo temperature of ~50 K.

9:36AM P12.00009 High field de Haas-van Alphen measurements of RT$_2$Zn$_{20}$ (R=Yb and Lu,T=Fe, Co and Rh)¹, N. NI, S. JIA, Ames Lab / Iowa State University, N. HARRISON, NMFL / Los Alamos, NM, G.D. SAMOLYUK, S.L. BUD’KO, P.C. CANFIELD, Ames Lab / Iowa State University — The de Haas-van Alphen (dHvA) effect in heavy fermion compounds YbFe$_2$Zn$_{20}$, YbCo$_2$Zn$_{20}$ and YbRh$_2$Zn$_{20}$, as well as the nonmagnetic compounds LuFe$_2$Zn$_{20}$, LuCo$_2$Zn$_{20}$ and LuRh$_2$Zn$_{20}$ have been observed in pulsed fields up to 55 T directed along [110] and in the temperature range 0.4K to 12K. The cyclotron effective masses of YbT$_2$Zn$_{20}$ (T=Fe,Co and Rh) range from 1.8m$_e$ to 2.8m$_e$. Self-consistent tight binding linear muffin-tin orbital method in the atomic sphere approximation (TB-LMTO-ASA) has been used to construct Fermi surfaces of LuT$_2$Zn$_{20}$ (T=Fe, Co and Rh). The calculated dHvA frequencies show good agreement with the experiments.

1Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

9:48AM P12.00010 Induced Phase Separation in GdBaCo$_2$Fe$_{2}$O$_{5.5-δ}$ by Fe Doping², YAN-KUN TANG, C.C. ALMASAN, Department of Physics, Kent State University, Kent, Ohio 44242, USA — A detailed magnetic study has been carried out for the Fe doped GdBaCo$_{2-δ}$Fe$_{2}$O$_{5.5-δ}$ (x = 0.02, 0.05, 0.10, and 0.20) cobaltites. Fe doping enhances the high temperature ferromagnetism present in the Fe-free samples and it induces a second ferromagnetic order, which develops at a lower T. Also, the spin-state transition temperature shifts to higher T with increasing the Fe content. Phase separation in two magnetic phases, namely, Fe-rich and Fe-free regions, provides a phenomenological interpretation of these magnetic behaviors. The Fe-rich regions are responsible for the second ferromagnetic order present at lower T. The shift of the low temperature M(T) peak related to this second ferromagnetic order is due to the decrease in the oxygen content in the Fe-rich regions with increasing Fe doping and the presence of the antiferromagnetic Fe-Co superexchange interaction in these regions. The high temperature M(T) peak (corresponding to the Fe-free regions) and the spin-state transition temperature shift to higher temperatures with Fe doping because of the slight compression of the Fe-free regions with Fe doping.

2This research was supported by the National Science Foundation under Grant No. DMR-0705959.

10:00AM P12.00011 Quantum Critical Phenomena in Ni$_3$Al$_{1-x}$Ga$_x$ Alloys³, M.H. FANG, Zhejiang University (ZJU) and Tulane University (TU), J.H. YANG, Z.A. XU, JZU, B. CHEN, Y. ITOH, K. YOSHIMURA, Kyoto University, Z.Q. MAO, TU — Considerable study has been devoted to quantum phase transitions (QPTs), which are believed to be a key concept for understanding the physics of strongly correlated electrons. In this talk we report on observation of quantum critical phenomena in Ni$_3$Al$_{1-x}$Ga$_x$ alloys. Ni$_3$Al is a ferromagnetic metal with T$_c$ = 41.5K. With Ga substitution for Al, T$_c$ and the spontaneous magnetic moment are gradually suppressed down to zero near the critical composition of $x_c$ ~ 0.4. We found that near the critical composition the magnetization as a function of magnetic field M(H) and the magnetic susceptibility as a function of temperature $\chi(T)$ both obey the scaling laws theoretically expected for QPTs, i.e., $M(H) \propto H^{1/3}$ and $\chi^{-1} \propto T^{4/3}$. In addition, we observed that near $x_c$ the derivative derived from the Arrott plots, i.e., $\gamma=d(M^2)/d(H/M)$ value exhibits a remarkable peak at about 2-3 T. This peak enhances with decreasing temperature. In terms of a recent theory, we argue that $\gamma$ reflects characteristics of spin excitation spectrum near QPTs.

3Work at Zhejiang University is supported by the PCSIRT of the Chinese Ministry of Education and Chinese 973 program (No. 2006CB601003) and work at Tulane University is supported by NSF, DOE.

10:12AM P12.00012 Physical properties of new ternary U compounds U$_3$Bi$_4$M$_3$ (M = Rh, Ni), TOMASZ KLIMCUK, HAN-OH LEE, FILIP RONNING, ERIC BAUER, TOMASZ DURAKIEWICZ, HEATHER VOLZ, JOE THOMPSON, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — A common belief has been that only Sb and Sn can form the U$_3$X$_4$M$_3$ structure. We have observed that also Bi can stabilize the structure as Ce$_3$P$_2$Bi$_4$, the well known Kondo insulator. Resistivity and photoemission spectroscopy measurements on U$_3$Bi$_4$N$_3$ indicate the presence of a charge gap, suggesting that it might be a Kondo insulator. However, the nonmagnetic reference compound Th$_3$Bi$_4$N$_3$ is a semiconductor, and, consequently, U$_3$Bi$_4$N$_3$ is rather a band insulator, similar to U$_3$Sb$_4$N$_3$. On the other hand, replacing Ni with Rh, which has one less electron than Ni, to form U$_3$Bi$_4$Rh$_3$ produces a metallic resistivity and modestly large electronic specific heat coefficient ($\gamma(0.4K) = 200 mJ/mol-U K^2$), characteristic of a Kondo-lattice system. Details of specific heat, magnetic susceptibility and electrical resistivity measurements on these single crystals will be discussed.

10:24AM P12.00013 Electronic and magnetic properties of single-crystalline UNi$_5$Sb$_2$,², B.K. DAVIS, M. S. TORIKACHVILI, Dep. of Physics, San Diego State U., E. D. MUN, J. C. FREDERICK, G. J. MILLER, S. THIMMAIAH, S. L. BUD’KO, P. C. CANFIELD, Ameslab and Iowa State U., G. M. SCHMIEDEHOFF, Dep. of Physics, Occidental C. — We studied the electronic and magnetic properties of antiferromagnetic UNi$_5$Sb$_2$ ($T_N \approx 161 K$) by means of measurements of magnetic susceptibility, thermal expansion, and electrical resistivity ($\rho$) at ambient pressure, and $\rho$ under hydrostatic pressures up to 20 kbar, in the temperature range from 1.9 to 300 K. The value of $\rho(T)/T$ changes drastically from positive below $T_N$ to negative above it, reflecting the loss of spin-disorder scattering in the ordered phase. Two small features in the $\rho$ vs $T$ data centered near 40 and 85 K, which are quite hysteresis in temperature, correlate well in temperature with features in the magnetic susceptibility, and thermal expansion. The effect of pressure is to suppress the amplitude of the small features in $\rho$ vs $T$ at lower temperatures, and to raise $T_N$ at the rate of $\approx 0.76 K/kbar$.

²Support from NSF Grant Nos. DMR-0306165 (SDSU), and DMR-0305397 (OC), and USDOE Contr. DE-AC02-07CH11358 (Ames and ISU) are gratefully acknowledged.
Tuning the ground state of CeNiGe$_3$ by applied magnetic field

8:00AM P13.00001 Energy and charge transfer in photoexcited molecules - A challenge for TDDFT

8:12AM P13.00002 Generator coordinates: a new road towards dynamics and excitations in DFT

8:24AM P13.00003 Time-Dependent Transport Phenomena: Bound-State Oscillations and Pumping

8:36AM P13.00004 Time-dependent V-representability on lattice systems

8:48AM P13.00005 TDDFT in Phase-Space

9:00AM P13.00006 Linear and Non-Linear Optical Response using Real-Time Time-Dependent Density Functional Theory

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

1Supported in part by NSF Grant 0120967 (YT) through the STC MDITR and DOE Grants DE-FG02-04ER15999 (FV) and DE-FG03-97ER45623 (JJR).

9:12AM P13.00007 Time-dependent density-functional approach for exciton binding energies\textsuperscript{1}, VOLODYMYR TURKOWSKI, CARSTEN A. ULLRICH, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211 — We use TDDFT to study ultrafast electron dynamics and excitonic effects in insulators and semiconductors. Within a two-band approximation of the linearized semiconductor Bloch equations, we derive a TDDFT version of the Wannier equation for excitonic wave functions and binding energies. The TDDFT Wannier equation produces in principle the exact excitonic spectrum. However, this puts stringent requirements on the exchange-correlation (XC) kernel. We analyze various XC kernels that lead to bound excitonic states, and propose new model XC kernels designed to reproduce experimental exciton spectra.

\textsuperscript{1}This work is supported by NSF Grant DMR-0553485.

9:24AM P13.00008 Autoionizing Resonances in TDDFT\textsuperscript{1}, HARSHANI WIJEWARDANE, AUGUST KRUEGER, GABRIELLA MULLADY, NEENA MAITRA, Hunter College of the City University of New York — In an independent-particle picture such as the Kohn-Sham system, bound states with an energy above one of the occupied orbital ionizations are truly bound. When interaction is accounted for, configuration coupling turns the bound state into an autoionizing resonance. In exact TDDFT, it is the exchange-correlation kernel that mixes the ionized and bound state, creating a Fano resonance profile. Although autoionization peaks arising from single excitations have been accurately captured with the available functional approximations, resonances arising from double excitations lying in the continuum are missing. By studying a simple model system, we uncover the features of the exact exchange-correlation kernel that are needed to capture the lifetimes and line shapes of these resonances accurately.

\textsuperscript{1}Supported by the National Science Foundation and the Research Corporation Cottrell Scholar Program


9:48AM P13.00010 Adiabatic connection fluctuation dissipation theorem density functionals beyond the random phase approximation, FILIPP FURCHE, University of California, Irvine — The random phase approximation (RPA) is an increasingly popular starting point for the construction of improved correlation energy functionals. As opposed to semi-local approximations, RPA-based functionals do not suffer from Coulomb self-interaction and naturally include van der Waals interactions; the price is higher computational cost. To compete with traditional correlated wavefunction methods, it is necessary to go beyond the bare RPA. I will analyze successes and failures of recent attempts to do so [1,2], and outline promising future directions. 


10:00AM P13.00011 New Perspectives on the Fundamental Theorem of Density Functional Theory\textsuperscript{1}, VIRAHT SAHNI, The Graduate School, CUNY, XIAO-YIN PAN, Ningbo University — The fundamental theorem of time-dependent/time-independent DFT due to Runge-Gross(RG)/Hohenberg-Kohn(HK) proves the bijectivity between the density $\rho(r)$ and the Hamiltonian $H(t)/H$ to within a function $C(t)/constant C$, and wave function $\Psi(t)/\Psi$. (Implicit in the RG theorem is that the initial condition $\Psi(t_0)$ is fixed.) As such in DFT the wave function is considered solely a functional of the density. Since the density is gauge invariant, the wave function as a functional of the density is also gauge invariant. However, it is well known that the Hamiltonian and wave function are gauge variant. There is, therefore, an inherent inconsistency in the RG/HK theorem. We resolve this inconsistency of the theorem via a unitary or equivalently a gauge transformation. As a consequence we generalize the theorem to external potentials that include the momentum operator and a curl-free vector potential operator. The RG/HK theorems then each constitute a special case of this generalization.

\textsuperscript{1}Supported in part by RF CUNY.

10:12AM P13.00012 Photo-excited dynamics of CH$_2$N$_2$; time-dependent density functional theory, HOSIK LEE, NEC Corp., YOSHIYUKI MIYAMOTO, NANO ELECTRONICS RESEARCH LABORATORIES, NEC CORPORATION TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM — A highly reactive organic molecule carbene has been an important subject in organic chemistry in several decades. The carbene which is formulated by R$_1$R$_2$C: shows high yield and lesser or no side products during its reaction [1]. By using ultra-fast (sub-pico second) laser flash photolysis(LFP) technique to its precursor diazirine or diazomethane, the highly reactive short-living (~100 fs) carbene can be conveniently prepared and used for production. In this study, photo-excited dynamics of diazirine and diazomethane will be shown within the scheme of the first principles time-dependent density functional calculations. With quite good agreements to experimental photo-excitation spectra, our preliminary calculation results show different phases of molecular motion which hardly is achieved with thermal effect. Temperature-induced kinetic effect in the photo-excited dynamics also is discussed.

10:24AM P13.00013 Time dependent density functional study of enhanced field emission from carbon nanotubes, JOSEPH DRISCOLL, KALMAN VARGA, Vanderbilt University, Nashville — We have calculated the field emission current of carbon nanotubes in real-time and real-space using the Lagrange- function basis [1] combined with efficient time-propagating schemes. Experimental studies reported orders of magnitude increase of field emission current from Cesium deposited carbon nanotubes [2]. We have studied the increase of field emission current due to the deposition of different atoms (Cesium, Gold, Tungsten, etc.) on capped carbon nanotube tips. The theoretical results are in good agreement with the experimental findings. This work was supported by NSF grant ECS 0522146.


Wednesday, March 12, 2008 8:00AM - 11:00AM –
Session P14 DBP BPS FIAP: High-Bandwidth Dynamic Atomic Force Microscopy  Morial Convention
Center 205

8:00AM P14.00001 High-Bandwidth Atomic Force Microscopy Reveals A Mechanical spike Accompanying the Action Potential in mammalian Nerve Terminals1, BRIAN M. SALZBERG, University of Pennsylvania School of Medicine — Information transfer from neuron to neuron within nervous systems occurs when the action potential arrives at a nerve terminal and initiates the release of a chemical messenger (neurotransmitter). In the mammalian neurohypophysis (posterior pituitary), large and rapid changes in light scattering accompany secretion of transmitter-like neuropeptides. In the mouse, these intrinsic optical signals are intimately related to the arrival of the action potential (E-wave) and the release of arginine vasopressin and oxytocin (S-wave). We have used a high bandwidth (20 kHz) atomic force microscope (AFM) to demonstrate that these light scattering signals are associated with changes in nerve terminal volume, detected as nanometer-scale movements of a cantilever positioning on top of the neurohypophysis. This method can be applied to any nervous system and may provide new insights into the mechanism(s) by which excitation is coupled to secretion at nerve terminals.

8:36AM P14.00002 Studying Chemical Reactions, One Bond at a Time, with Single Molecule AFM Techniques, JULIO M. FERNANDEZ, Department of Biological Sciences, Columbia University, New York, NY 10027, USA — The mechanisms by which mechanical forces regulate the kinetics of a chemical reaction are unknown. In my lecture I will demonstrate how we use single molecule force-clamp spectroscopy and protein engineering to study the effect of force on the kinetics of thiol/disulfide exchange. Reduction of disulfide bond via the disulfide/disulfide exchange chemical reaction is crucial in regulating protein function and is of common occurrence in mechanically stressed proteins. While reduction is thought to proceed through a substitution nucleophilic bimolecular (SN2) reaction, the role of a mechanical force in modulating this chemical reaction is unknown. We apply a constant stretching force to single engineered disulfide bonds and measure their rate of reduction by dithiothreitol (DTT). We find that while the reduction rate is linearly dependent on the concentration of DTT, it is exponentially dependent on the applied force, increasing 10-fold over a 300 pN range. This result predicts that the disulfide bond lengths by 0.34 Å at the transition state of the thiol/disulfide exchange reaction. In addition to DTT, we also study the reduction of the engineered disulfide bond by the E. coli enzyme thioredoxin (Trx). Thioredoxins are enzymes that catalyze disulfide bond reduction in all organisms. As before, we apply a mechanical force in the range of 25-450 pN to the engineered disulfide bond substrate and monitor the reduction of these bonds by individual enzymes. In sharp contrast with the data obtained with DTT, we now observe two alternative forms of the catalytic reaction, the first requiring a reorientation of the substrate disulfide bond, causing a shortening of the substrate polypeptide by 0.76±0.07 Å, and the second elongating the substrate disulfide bond by 0.21±0.01 Å. These results support the view that the Trx active site regulates the geometry of the participating sulfur atoms, with sub-Ångström precision, in order to achieve efficient catalysis. Single molecule atomic force microscopy (AFM) techniques, as shown here, can probe dynamic rearrangements within an enzyme’s active site which cannot be resolved with any other current structural biological technique. Furthermore, our work at the single bond level directly demonstrates that thiol/disulfide exchange in proteins is a force-dependent chemical reaction. Our findings suggest that mechanical force plays a role in disulfide reduction in vivo, a property which has never been explored by traditional biochemistry.

9:12AM P14.00003 Imaging and Beyond with High Speed AFM, PAUL HANSMA, University of California at Santa Barbara — It is now possible to perform AFM experiments at speeds of up to 600 lines per second over scan ranges exceeding 10 microns. For a 100 x 100 pixel image this gives frame rates of 60 frames/second: faster than video rate. This has required small cantilevers, new scanners, new high voltage amplifiers, and a new scan control system. The small cantilevers are from SCL Sensor-Tech (Deutsch-Wagram, Austria). The new scanner is based on a sophisticated system of flexures that constrain the motion of each separate piezo stack to one dimension in a three-dimensional scanner. It has a scan range of 15 microns and a lowest resonance frequency of about 27 kHz. The new high voltage amplifier, built in collaboration with TechProject (Vienna, Austria), can deliver up to 8 amps over the entire output range from 0 to 150 volts with the challenge of having the piezo as a capacitive load. The new scanner is based around a commercially available DAQ board in a Windows environment. One of the major challenges is now to move beyond imaging to Force-Volume imaging, which involves taking an array of force curves over a sample and then reconstructing a zero force image as well as a map of local mechanical properties.

9:48AM P14.00004 AFM probes with integrated electrostatic actuators for fast, quantitative imaging and force spectroscopy, LEVENT DEGERTEKIN, Georgia Institute of Technology — In this talk, we summarize our efforts in developing novel AFM probes (FIRAT) with integrated sensing and actuation. These probes exploit recent advances in microscale sensor technology and open up the design space for AFM applications including fast imaging, quantitative material characterization and single molecular mechanics measurements. For fast imaging applications in air, probes with aluminum force sensing structures are surface micromachined on quartz substrates. Using 0.7-0.8µm thick, 40µm x 60µm clamped-clamped beams over 2.8µm of air gap, probes with resonance frequencies in the order of 1MHz and Q in the 5-15 range are obtained. These probes are actuated directly by electrostatic forces applied to the mechanical structure by rigid electrodes on the substrate shaped as optical diffraction gratings, enabling imaging bandwidths in the order of 100kHz. The integrated grating interferometer provides 10fm/√Hz level displacement sensitivity down to 3Hz. The surface micromachining approach used for probe fabrication lets one to precisely control the probe dynamics and overcome the difficulties associated with regular AFM cantilevers for applications such as time resolved interaction force (TRIF) measurements. Using FIRAT probes with over damped dynamics, clean TRIF signals are obtained while imaging the surface at regular speeds. This enables us to use a simple model to invert quantitative mechanical properties of a variety of polymers. For measurements on single molecules, membrane type FIRAT probes suitable for in liquid operation have been developed. These probes are made of dielectric materials with embedded actuation electrodes. Used only as actuators or both actuators and force sensors, these devices are shown to enable parallel force spectroscopy measurements. We also show that the spring constant of these probes can be electrically reduced to achieve higher force sensitivity while not affecting its noise performance and discuss the effect of hydrodynamic forces in these membrane type probes as compared to cantilever type probes for fast force spectroscopy measurements.

1Supported by USPHS grant NS40966
2Supported by NIH RO1 GM 065354-05 and Veeco
3This work is supported by US NSF and NIH
10:24AM P14.00005 High-speed AFM for Studying Dynamic Biomolecular Processes. This work was supported by CREST/JST.

Wednesday, March 12, 2008 8:00AM - 11:00AM – Session P15 GQI: Focus Session: Superconducting Qubits II Morial Convention Center 207

8:00AM P15.00001 Quantum non-demolition measurement of a superconducting two-level system. ADRIAN LUPASCU, Kavli Institute of NanoScience, Delft University of Technology, The Netherlands — In quantum mechanics, measurement can be understood as the interplay between extraction of information and disturbance of the state of the measured system. For projective measurements this disturbance is minimized: the post-measurement state is fully correlated to the indication of the detector. Quantum non-demolition (QND) detection is a strategy used to implement a projective measurement, which relies on a specific type of interaction between the measured system and the detector. In our experiments we apply these principles to the measurement of a superconducting flux qubit, which is an artificial two-level system built using mesoscopic Josephson junctions. Our detection method relies on probing the response of a hysteretic non-linear resonator coupled to the qubit. This setup allows for very efficient detection of the state of our system, with a measured contrast of 85%. The large correlations between the results of two consecutive measurements demonstrate the QND nature of this method. This result establishes the validity of a QND strategy for projective measurement of superconducting qubits and has implications for quantum information processing.

8:36AM P15.00002 Tunneling of a modulated oscillator: quantum interference in the classically forbidden region. MICHAEL MARTHALER, MARK DYKMAN, Michigan State University — We describe a new coherent quantum effect in periodically modulated systems. It occurs in a modulated nonlinear oscillator and has no analog in two-level systems. The effect consists in oscillations and sign change, with the varying modulation frequency, of the tunnel splitting of the symmetric and antisymmetric time-periodic states. These states are formed by period-2 oscillator states, which classically have the same amplitudes and opposite phases. The effect is due to the wave function oscillations and the related interference in the classically forbidden region of the oscillator phase space. The tunnel splitting oscillations emerge already in the “ground state” of the oscillator Hamiltonian in the rotating frame. The WKB analysis in the rotating wave approximation is in excellent agreement with the numerical results. The tunnel splitting oscillations persist in the parameter range where the rotation wave approximation becomes inapplicable. The effect occurs in the parameter range accessible with currently available Josephson junction-based systems.

9:00AM P15.00004 Measurement induced heat bath and decay rates in circuit QED. MAXIME BOISSONNEAULT, Université de Sherbrooke, JAY GAMBITTA, IQC, University of Waterloo, ALEXANDRE BLAIS, Université de Sherbrooke, YALE CIRCUIT QED TEAM — In circuit QED, a superconducting qubit is fabricated inside a high quality superconducting coplanar resonator. This system allows for strong interaction of the artificial atom with the photon field [1]. In the dispersive regime, where the detuning between the qubit and the resonator frequency is large with respect to their coupling, the physics of this system is understood in terms of Lamb and Stark shifts. However, as the coupling strength or the number of photons in the resonator increases, this description breaks down. In this talk, we will explain that, when taking into account higher order corrections to the dispersive approximation, measurement photons act as a heat bath inducing incoherent relaxation and excitation of the qubit. We will discuss how this can decrease achievable signal-to-noise ratio and may reduce the QND aspect of the measurement. [1] A. Wallraff, et al., Nature 431, 162 (2004)

9:12AM P15.00005 Single shot readout in a circuit QED system. ANDREW HOUCK, Yale University, ALEXANDRE BLAIS, Université de Sherbrooke, STEVEN GRIVIN, ROBERT SCHOELKOPF, Yale University — In the dispersive limit of circuit QED, measurement-induced decoherence can be used for quantum non-demolition measurements of the state of a superconducting qubit. Here, we present an optimization of the measurement of a transmon qubit, including a new understanding of how measurement affects the rate of demolition. Both cavity and qubit parameters were optimized to maximize signal to noise without introducing substantial new channels for decoherence. Single shot readout fidelities of over 70% have been achieved, and greater than 90% fidelity should be possible with presently achievable coherence times. This opens up the possibility of observing quantum jumps in the state of the qubit. Work done in collaboration with the Yale circuit QED team.
9:24AM P15.00006 Dissipation and cooling of a nanomechanical oscillator coupled to a Cooper pair box1, RAKESH TIWARI, D. STROUD, Department of Physics, The Ohio State University — We calculate the dynamics of a nanomechanical oscillator (NMO) coupled capacitively to a Cooper pair box (CPB), by solving a stochastic Schrodinger equation with two Lindblad operators. Both the NMO and the CPB are assumed dissipative. We show numerically that, if the CPB decay time is smaller than the NMO decay time, the coupled NMO will lose energy faster, and the coupled CPB more slowly, than the uncoupled NMO and CPB. We find that both of these effects are largest if 3 times the NMO frequency equals the energy splitting of the CPB. Thus we show that an NMO can be cooled to low temperatures much more efficiently by coupling the NMO to a CPB.

1This work is supported by NSF DMR04-13395.

9:36AM P15.00007 Microwave Reflectometry Measurements of Flux States of a dc SQUID Phase Qubit1, B. K. COOPER, R. M. LEWIS, S. K. DUTTA, T. A. PALOMAKI, ANTHONY PRZYBYSZ, H. KWON, HANHEE PAIK, J. R. ANDERSON, C. J. LOBB, F. C. WELLSTOOD — We performed measurements of a 2-junction niobium circuit in a dc-SQUID configuration, with near zero current bias and flux bias close to half a flux quantum. Because of the large self-inductance, the potential of an intrinsic phase qubit has several minima. In order to perform quantum operations from a single well, a technique using low-frequency microwaves is presented. Due to the large self-inductance, the potential of an intrinsic phase qubit has several minima. In order to perform quantum operations from a single well, a technique using low-frequency microwaves is presented.

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The utility of this measurement for qubit state readout is discussed.

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Our device is a Nb/AlOx/Nb SQUID fabricated by Hypres with loop inductance of 1.3 nH and symmetric junction critical currents of approximately 5 µA. The SQUID is current and flux biased, with one junction used as the qubit and the other used to provide isolation. The isolation junction is shunted by a large capacitor to depress its plasma frequency to about 1.5 GHz. This frequency can be shifted by flux-induced circulating current in the SQUID loop, allowing us to determine which flux state we are in by making reflectometry measurements of the resonant behavior of the isolation junction. The utility of this measurement for qubit state readout is discussed.

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We will discuss how the measurement performance depends on biasing parameters of each junction.

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1Fundring from the Joint Quantum Institute and the NSA.

9:48AM P15.00008 Measurements of a dc-SQUID phase qubit using rf-reflectometry1, R.M. LEWIS, University of Maryland, B.K. COOPER, S.K. DUTTA, T. A. PALOMAKI, HANHEE PAIK, A. PRZYBYSZ, H. KWN, J. R. ANDERSON, C. J. LOBB, F. C. WELLSTOOD — We performed measurements of a Nb/AlOx/Nb dc-SQUID phase qubit at 100 mK by monitoring the plasma frequency, fp, of the readout/isolation junction. This qubit contains two Josephson junctions (JJs) separated by a 1.3 nH inductance; one JJ operates as a pure phase qubit, the second JJ isolates and reads out the qubit junction. When driving the isolation junction at 1.5 GHz near fp, current fluctuations in the SQUID loop cause fluctuations in fp, which appear in the sidebands of the reflected microwave power. At 100 mK we find an effective flux noise, Sθ2/2 of 50 µµ0/Hz1/2 at 1 Hz. The measurement bandwidth is about 10 MHz, the upper limit being set by the Q of the readout junction. We will discuss how the measurement performance depends on biasing parameters of each junction.

1Supported by the E.U. through the EuroSQIP project.

10:00AM P15.00009 DC SQUID Phase Qubit with LC Filter, HYEOKSHIN KWON, A.J. PRZYBYSZ, HANHEE PAIK, R. M. LEWIS, T. A. PALOMAKI, S.K. DUTTA, B.K. COOPER, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, University of Maryland, College Park — We investigate the use of an inductor-capacitor (LC) network to increase the isolation of a dc SQUID phase qubit from its current bias leads and thereby increase the dissipation time T2 and coherence time T1. One junction in the SQUID acts as an ideal phase qubit while the second junction and the SQUID loop inductance act as a broadband filter to isolate the first junction from the current bias leads. The LC-isolation network provides an additional isolation factor and allows flexibility in the choice of SQUID parameters. In addition to increasing the isolation from the leads, our design minimizes the effects of dielectric loss and two-level systems by using a relatively small Josephson junction, building the devices from Al/AlOx/Al on sapphire, and only using insulating layers (SiNx) in external capacitors for the readout junction and LC network. *Funding provided by JQI, CNAM and the DOD.

10:12AM P15.00010 Strong tunable coupling between a charge qubit and a phase qubit1, AURELIEN FAY, EMILE HOSKINSON, FLORENT LECOCQ, LAURENT LEVY, Institut Neel, CNRS-UJF, FRANK HEKKING, LPMMC, CNRS-UJF, WIEBKE GUICHARD, OLIVIER BUISSON, Institut Neel, CNRS-UJF. — We have studied the quantum dynamics of a superconducting circuit based on a dc-SQUID coupled to a highly asymmetric Cooper pair transistor (ACPT). The dc-SQUID is a phase qubit controlled by a bias current and magnetic field. The ACPT is a charge qubit controlled by a bias current, magnetic flux and gate voltage. We have measured by microwave spectroscopy the lowest quantum levels of the coupled circuit as function of applied flux, bias current and gate voltage. Quantum state measurements of the phase and charge qubit are achieved by a nanosecond flux pulse applied to the dc-SQUID. Our circuit enables the independent manipulation of each qubit as well as the entanglement of the quantum states of the two circuits. We observe avoided level crossings between the two qubits when they are put in resonance. The coupling strength is measured over a large frequency range and varies from 100MHz to 1.3GHz. We succeed to realize a tunable coupling between the charge and the phase qubit. The measured tunable coupling strength is well explained by a combination of a capacitive and a Josephson coupling between the two qubits.

1Supported by the E.U. through the EuroSQIP project.

10:24AM P15.00011 Superconducting phase qubit in a “camel” potential1, EMILE HOSKINSON, FLORENT LECOCQ, AURÉLIEN FAY, NICOLAS DIDIER, Institut Neel and LPMMC, CNRS-UJF, Grenoble, France, RALF DOLATA, ALEXANDER ZORIN, PTB, Braunschweig, Germany, FRANK HEKKING, WIEBKE GUICHARD, OLIVIER BUISSON, Institut Neel, CNRS-UJF, Grenoble, France — A prototypical phase qubit consists of a single current biased Josephson junction, in which the dynamics of the phase across the junction is analogous to a quantum particle trapped in a quadratic-cubic potential. We demonstrate a phase qubit in a double barrier quadratic-quartic “camel” potential. This potential is formed by a 2-junction niobium circuit in a dc-SQUID configuration, with near zero current bias and flux bias close to half a flux quantum. Because of the symmetry of the potential, the qubit is predicted to be optimally insensitive to current fluctuations. We perform a nanosecond single shot measurement by applying a flux pulse which reduces the height of the two potential barriers, allowing the excited state of the qubit to escape by two independent paths to an adjacent flux state of the dc-SQUID. We find Rabi oscillation, Ramsey oscillation, and energy relaxation decay times on the order of 60 ns, 20 ns, and 100 ns, respectively. Via spectroscopy, we show that the effects of current noise are rendered negligible in this circuit.

1Supported by the EU through the EuroSQIP project.

10:36AM P15.00012 Properties of a High-Tc Intrinsic Phase Qubit, X. Y. JIN, J. LISENFELD, Y. KOVAL, A. V. USTINOV, P. MÜLLER, Physics Department, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-91058, Erlangen, Germany — We discuss the properties of high-Tc intrinsic phase qubits. An intrinsic phase qubit is a superconducting ring made of a Bi2Sr2CaCu2O8+δ single crystal, intercepted by two intrinsic Josephson junction stacks. As a stack consists of many intrinsic Josephson junctions, an intrinsic phase qubit can be regarded as a multi-junction system, i.e. a system of many degrees of freedom in phase space. However, I-V characteristics and switching current distributions of our samples show that an intrinsic phase qubit behaves like a system with only two degrees of freedom, independent of the number of junctions in the stacks, as long as the two stacks are uniform. Due to the large self-inductance, the potential of an intrinsic phase qubit has several minima. In order to perform quantum operations from a single well, a technique using low-frequency microwaves is presented.
Performing a linear stability analysis of the actin velocity due to perturbations of the fragment boundary, we find that as the dimensionless profile is radial and is imposed by mass conservation for constant polymer density. The radius of the fragment is fixed by conservation of total monomer and start moving. In the stationary state in our model, actin polymerizes at the fragment edge and depolymerizes uniformly in the bulk. The initial velocity lies is sufficiently strong. The motivation for this work are the experiments of Verkhovsky et al. (Verkhovsky et al, Curr. Biol., 9: 11-20 (1999)) in which flat, circular, stationary cell fragments on a substrate, containing only actin and myosin motors, can either spontaneously or under applied force change shape and start moving. In the stationary state in our model, actin polymerizes at the fragment edge and depolymerizes uniformly in the bulk. The initial velocity profile is radial and is imposed by mass conservation for constant polymer density. The radius of the fragment is fixed by conservation of total—monomer and filamentous—actin. Performing a linear stability analysis of the actin velocity due to perturbations of the fragment boundary, we find that as the dimensionless parameter $\frac{\xi R_0^2}{\eta} \rightarrow 0$, where $\xi$ is the actin-substrate friction, $\eta$ is the viscosity, and $R_0$ is the initial fragment radius, the perturbed velocity obeys a Darcy Law, and combined with the force-free condition at the fragment boundary, this leads identically to a viscous fingering instability. This asymptotic limit should be achievable since $R_0$ can be tuned by making a fragment with enough actin.

The interaction between severing and annealing in disassembling a model lamellipodial actin network. The network is treated as a periodic array of crosslinked actin filaments which sever randomly. The lamellipodial actin density drops abruptly as a function of distance from the membrane in the absence of annealing. When annealing is included, the drop is more gradual, and at a critical value of the annealing rate the thickness becomes infinite. It is shown that lamellipodial disassembly is controlled by two characteristic times: the time that a single subunit remains in the network, and the time that it takes for actin polymerized at the membrane to move to the edge of the lamellipodium.

Supported by the National Science Foundation under grant DMS-0240770.

The stochastic dynamics of filopodial growth. We have investigated the length distribution of individual filaments in a growing filopodium and studied how it depends on various physical parameters. The distribution of filament lengths turned out to be narrow, which we explained by the negative feedback created by the membrane load and monomeric G-actin gradient. We also discovered that filopodial growth is strongly diminished upon increasing retrograde flow, suggesting that regulating the retrograde flow rate would be a highly efficient way to control filopodial extension dynamics. The filopodial length increases as the membrane fluctuations decrease, which we attributed to the unequal loading of the membrane force among individual filaments, which, in turn, results in larger average polymerization rates. We also observed significant diffusional noise of G-actin monomers, which leads to smaller G-actin flux along the filopodial tube compared with the prediction using the diffusion equation.

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Mechanics of Lamellipodia. The actin cytoskeleton is a morphologically-complex assembly of cross-linked F-actin filaments. The cytoskeleton provides rigidity for the cell within appropriate time scales so that it can change its shape to, for example, crawl along surfaces. In addition to cross-linking proteins, many other proteins are involved in the assembly of the actin cytoskeleton such as branching proteins, capping proteins, and severing proteins. Presumably these proteins work cooperatively toward the dynamic formation of rigidity. We will initially focus on the role of branching proteins. The F-actin filaments in lamellipodia—protrusions of the mobile edge of a crawling cell—have some overall orientation due to the branching. Branched filaments emerge at a 70 degree angle from the mother filament’s growing end. This overall orientation is modelled as an anisotropy in an effective medium theory determining the cytoskeleton’s elasticity in the static regime. The potential for a splay rigid phase, in addition to a rigid phase, is also investigated.

The stochastic dynamics of filopodial growth. We have investigated the length distribution of individual filaments in a growing filopodium and studied how it depends on various physical parameters. The distribution of filament lengths turned out to be narrow, which we explained by the negative feedback created by the membrane load and monomeric G-actin gradient. We also discovered that filopodial growth is strongly diminished upon increasing retrograde flow, suggesting that regulating the retrograde flow rate would be a highly efficient way to control filopodial extension dynamics. The filopodial length increases as the membrane fluctuations decrease, which we attributed to the unequal loading of the membrane force among individual filaments, which, in turn, results in larger average polymerization rates. We also observed significant diffusional noise of G-actin monomers, which leads to smaller G-actin flux along the filopodial tube compared with the prediction using the diffusion equation.

Mechanics of Lamellipodia. The actin cytoskeleton is a morphologically-complex assembly of cross-linked F-actin filaments. The cytoskeleton provides rigidity for the cell within appropriate time scales so that it can change its shape to, for example, crawl along surfaces. In addition to cross-linking proteins, many other proteins are involved in the assembly of the actin cytoskeleton such as branching proteins, capping proteins, and severing proteins. Presumably these proteins work cooperatively toward the dynamic formation of rigidity. We will initially focus on the role of branching proteins. The F-actin filaments in lamellipodia—protrusions of the mobile edge of a crawling cell—have some overall orientation due to the branching. Branched filaments emerge at a 70 degree angle from the mother filament’s growing end. This overall orientation is modelled as an anisotropy in an effective medium theory determining the cytoskeleton’s elasticity in the static regime. The potential for a splay rigid phase, in addition to a rigid phase, is also investigated.
9:24AM P16.00006 Nonlinear elasticity of composite networks of stiff biopolymers with flexible linkers. CHASE BROEDERSZ, Vrije Universiteit, C. STORM, Vrije Universiteit and Universiteit Leiden, F. C. MACKINTOSH, Vrije Universiteit — Motivated by recent experiments showing novel rheological properties of biopolymer networks, we develop an effective medium theory for rigid filaments cross-linked by flexible linkers. Specifically, we treat such a network as a collection of randomly oriented stiff polymers mechanically connected by highly compliant cross-linkers to an elastic continuum, which effectively represents the surrounding network. For cross-links with a finite compliance, we find a smooth cross-over between two distinct elastic regimes. Starting from a linear elastic regime dominated by cross-link elasticity, the network begins to stiffen significantly as the cross-links reach full compliance. We extend this model to a self-consistent one, in which the effective medium reflects the non-linear elastic properties of the cross-linked network. This model yields a cross-over to a nonlinear regime that is consistent with recent experimental studies of the cellular cytoskeletal polymer F-actin with filamin cross-links. 


9:36AM P16.00007 Effects of Osmotic Force and Torque on Microtubule Bundling and Pattern Formation. YONGXING GUO, YIFENG LIU, Physics Department, Brown Univ., RUDOLF OLDENBOURG, Marine Biological Laboratory, JAY TANG, JAMES VALLES, Physics Department, Brown Univ. — We report the effect of Polyethylene Glycol (PEG, MW=35kd) on microtubule bundling and pattern formation. Without PEG, polymerizing microtubule (MT) solutions of a few mg/ml [1,2] can spontaneously form striated birefringence patterns through MT alignment, bundling and buckling in coordination. With PEG, bundles become more distinct and the birefringence pattern weakens. Using quantitative birefringence measurements, the average number of MTs in the cross section of a bundle induced by 1% w/w PEG 35kd is determined to be around 26, with a wide spread in size. The amplitude of the buckling is reduced with increased PEG concentration. At sufficiently high PEG concentration (0.5% w/w), the pattern is totally suppressed and the sample contracts laterally during the development of a microtubule bundle network. We propose that the decrease of the buckling amplitude is due to the depletion of the dispersed MT network, which is essential for the pattern formation. We attribute the anisotropic contraction to an osmotic torque that drives bundles that cross to align. [1] Y. Liu, et al, PNAS 103, 10654 (2006). [2] Y. Guo, et al, PRL 98, 198103 (2007). [Supported by NASA (NNA04CC57G, NAG3-2882) and NSF (DMR 0405156)]

9:48AM P16.00008 Buckling and force propagation in intracellular microtubules. MOUMITA DAS, Vrije Universiteit, ALEX J. LEVINE, University of California, Los Angeles, F. C. MACKINTOSH, Vrije Universiteit — Motivated by recent experiments [1] showing the buckling of microtubules in cells, we study theoretically the mechanical response of, and force propagation along elastic filaments embedded in a non-linear elastic medium. We find that embedded microtubules buckle when their compressive load exceeds a critical value \( f_c \), which is two orders of magnitude larger than for an isolated MT as found earlier [1], and that the resulting deformation is restricted to a penetration depth that depends on both the non-linear material properties of the surrounding cytoskeleton, as well as the direct coupling of the microtubule to the cytoskeleton possibly through MT-associating proteins (MAPs). The deformation amplitude depends on the applied load \( f > f_c \), as \( (f-f_c)^{1/2} \). This work shows how the range of compressive force transmission by microtubules can be as large as tens of microns, and is governed by the mechanical coupling to the surrounding cytoskeleton.

References:

10:00AM P16.00009 Hydrodynamic tether extrusion from “gelly” vesicles. KARINE GUEVORKIAN, SEBASTIEN KREMER, FRANCOISE BROCHARD-WYART, Institut Curie — Extrusion of cell tethers requires the detachment of the plasma membrane and GPI used to probe the forces generated by membrane-cytoskeleton adhesion. We have studied the hydrodynamic extrusion of tethers from red blood cells [1] and developed a theoretical model based on permeation of lipids through the network of membrane proteins linked to the cytoskeleton [2]. Our aim here is to probe the model on biomimetic systems, namely lipid vesicles filled with artificial cytoskeleton made of synthetic or biological gels, where we can adjust the membrane-cytoskeleton coupling. The properties of tubes extruded from these “gelly” vesicles will be compared to simple vesicles on one hand, and to red blood cells or human carcinoma BON cells on the other. [1] N. Borghi et al, Biophys. J. 93 (2007) [2] F. Brochard-Wyart, et al, Proc. Natl. Acad. Sci. USA, 103 (2006)

10:12AM P16.00010 Living Microlens Arrays. JESSICA ZIMBERLIN, PATRICIA WADSWORTH, ALFRED CROSBY, University of Massachusetts — Using the properties of living cells and early tissue formation, we define adaptable surface structures of three-dimensional, hexagonal arrays of microchannels. These “living” microchannels are achieved by growing a monolayer cell sheet on a thin film of poly(ethylene) [PS] attached to a substrate of crosslinked poly(dimethyl siloxane) [PDMS] microwells. The contractile nature of the cells attached to the surface and the compliance of the PDMS surface geometry allows the PS thin film to buckle, forming arrays of convex microchannels. The curvature of the microchannels is related to the strain applied by monolayer cell sheets to the PS surface. We use this measurement to differentiate the strains applied by two different cell types and relate these strains to differences in the intercellular coupling of the different cell types. We also show that by adding different chemical triggers to the system, the contractile nature of the cells changes, modifying the focal length of the microchannels. This design introduces a new paradigm for advanced materials and offers great promise for a range of applications.

1 Authors would like to acknowledge NSF-IGERT and NIH for their support.

10:24AM P16.00011 Local viscoelasticity of the surfaces of individual Gram-negative bacterial cells measured using atomic force microscopy. VIRGINIA VADILLO-RODRIGUEZ, TERRY BEVERIDGE, JOHN DUTCHER, University of Guelph — The cell wall of Gram-negative bacteria performs many important biological functions: it plays a structural role, it allows the selective movement of molecules across itself, and it allows for growth and division. These functions not only suggest that the cell wall is dynamic, but that its mechanical properties are very important. We have used a novel, AFM-based approach to probe the mechanical properties of single bacterial cells by applying a constant compressive force to the cell under physiological conditions while measuring the time-dependent displacement (creep) of the AFM tip due to the viscoelastic properties of the cell. For these experiments, we chose a representative Gram-negative bacterium, E. coli (E. coli) PA01, and we used AFM tips of different size and geometry. We find that the cell response is well described by a three element mechanical model with an effective cell spring constant \( k \) and an effective time constant \( \tau \) for the creep motion. Adding glutaraldehyde, which increases the covalent bonding of the cell surface, produced a significant increase in \( k \) and a significant decrease in \( \tau \).

10:36AM P16.00012 Stall Force and Response of Lung Cilia. RICHARD SUPERFINE, DAVID HILL, VINAY SWAMINATHAN, E. TIMOTHY O’BRIEN, University of North Carolina, RIC BOUCHER, BRIAN BUTTON, ASHLEY ESTES — We report on the response of lung cilia to applied forces. We have applied magnetic forces to magnetic beads attached to individual human lung cilia in cell cultures. Our magnetic system is capable of generating large forces (~1 nanoNewton on 1 micron beads) with a 3kHz bandwidth. We record the cilium beat motion using video microscopy to record beat frequency and amplitude as a function of applied force. We present three major findings. First, the stall force is approximately 150 pN. Second the frequency is unchanged by the application of forces up to the stall point. Third, the speed of the beat motion slows down according to the diminution of the beat amplitude while maintaining a constant frequency and the speed of the motion is the same whether the beat direction is in the same direction as the applied force or against the applied force.
8:00AM P17.00001 Simulating the Melting Transition of Helium in Two Dimensions . KEOLA WIERSCHEM, MARTECH & Dept. of Physics, Florida State University, EFSTRATIOS MANOUSAKIS, MARTECH & Dept. of Physics, Florida State University, and Dept. of Physics, University of Athens, Greece — We study the melting behavior of $^4\text{He}$ in two dimensions with the path integral Monte Carlo method. Systems of helium atoms are simulated in a periodic cell designed to accommodate a triangular solid. We calculate the translational and orientational order parameters, as well as the defect fraction. Defects are defined as atoms with more or less than six neighbors; the nearest neighbor network is found through Delaunay triangulation. Two dimensional melting is a defect-mediated phase transition, thus, defects will proliferate as the solid is melted. Additionally, melting is expected to occur via a two-stage process, with transitions for both translational and orientational order. At high number density (0.0846 Å$^{-2}$), we have seen a single transition (within the accuracy of our simulations). We are currently working to observe the melting transition at lower densities.

8:12AM P17.00002 Lithium, magnesium and sodium $^4\text{He}$ adsorption experiments performed below 1K. ELI VAN CLEVE, PETER TABOREK, JAMES RUTLEDGE, University of California, Irvine — We have constructed a $^4\text{He}$ optical cryostat and used a previously developed technique of Cryogenic Pulsed Laser Deposition (CPLD) (1), to deposit films of sodium, lithium and magnesium onto the surfaces of quartz crystal microbalances at cryogenic temperatures. The elements in the first and second column of the periodic table interact weakly with adsorbed helium. Theoretical calculations predict that helium will wet all the elements lighter than rubidium, but solid-like layers will not form, so liquid and superfluid films can exist at sub-monolayer coverage. We will present vapor pressure isotherms on Li, Mg and Na substrates in the temperature range 0.5K -1.3K and discuss the wetting and superfluid onset behavior. We will also present in-situ optical work function measurements of the metallic films, and discuss the relation between work function and wettabillity. (1) E. Van Cleve, P. Taborek, J.E. Rutledge JLTP online

8:24AM P17.00003 Third Sound Propagation in Superfluid $^4\text{He}$ Films Adsorbed on Nanotube Bundles . SONNY VO, TIM HSIEH, JOHN SCHULMAN, GARY A. WILLIAMS, UCLA — We have observed the propagation of third sound waves in thin superfluid $^4\text{He}$ films adsorbed on carbon nanotube bundles. The nanotubes are sprayed onto a plexiglass substrate, forming a tangle of interconnected bundles that is about 15 μm thick and 2.5 cm square, with an average bundle diameter of about 4 nm. A heater and bolometer at opposite corners allow detection of resonant third sound modes, and the third sound speed is deduced from the resonant frequencies. The helium adsorption is greatly affected by the surface tension forces generated by the high curvature of the nanotubes, and the film thickness on the tubes remains very thin compared to the thickness in flat regions of the cell. As helium is metered into the cell at 1.3 K the Kosterlitz-Thouless transition on the nanotubes is observed as the onset of the third sound signal, and then with increasing film thickness the third sound velocity decreases. The velocity appears to be dropping towards zero at a finite film thickness. In flat regions of the tube, in qualitative agreement with a surface-tension instability predicted for cylindrical geometries by Cole and Saam [Phys. Rev. Lett., 32, 985 (1974)].

3Work supported by the NSF, DMR 05-48521. We thank D. Hecht and G. Gruner for preparing the nanotubes.

8:36AM P17.00004 Bose-Einstein Coherence in Two Dimensional Superfluid $^4\text{He}$ . SOULEYMANE DIALLO, University of Delaware, JONATHAN PEARCE, National Physical laboratory, UK, RICHARD AZUAH, NIST Center for Neutron Research, JON TAYLOR, Rutherford Appleton Laboratory, HENRY CLEVE, University of Delaware — We present high-resolution measurements of the momentum distribution of atoms in liquid $^4\text{He}$ films adsorbed in nanoporous MCM-41, with 45 Å mean pore diameter. The measurements were performed at temperatures $T = 0.3$ K and $T = 2.3$ K and saturated vapor pressure (SVP) in the wavevectors range $32 < Q < 29$ Å$^{-1}$ using the MARI time-of-flight (TOF) chopper spectrometer at the ISIS spallation neutron source. The main goal is to determine whether there is a Bose-Einstein condensate (or coherence) in a finite-size two dimensional (2D) Bose fluid at low temperatures. It is also to investigate the 2D-3D dimensional crossover in the condensate properties. We find clear evidence of a condensate parameter, $n_0$, at $T = 0.3$ K in the films investigated. In the thinnest film (~approximately one atomic layer thick), the observed condensate fraction is greater than but consistent with the bulk superfluid 4He value of 7.25% within precision; i.e. $n_0 = (9.34 \pm 3.84)\%$. As more $^4\text{He}$ is adsorbed in the substrate pores, $n_0$ appears to decrease below the bulk value, possibly due to the disorder introduced by the confining media; i.e. $n_0 = (2.45 \pm 2.54)\%$ near full pore filling.

8:48AM P17.00005 Dynamics of one and two dimensional solid $^4\text{He}$ adsorbed on nanotubes . BJORN FAK, CEA, DRFMC Grenoble, France, SOULEYMANE DIALLO, University of Delaware, MARK ADAMS, Rutherford Appleton Laboratory, UK, OSCAR VILCHES, University of Washington, HELMUT SCHOBER, Institut Laue Langevin, Grenoble, France, HENRY GLYDE, University of Delaware — In a previous experiment[1], we showed that one dimensional (1D) solid helium can be created on the surface of nanotube bundles. Specifically, when $^4\text{He}$ is first adsorbed on nanotubes, it forms a 1D linear solid along the grooves between two nanotubes on the bundle surface with lattice parameter, $a_1 = 3.40 \pm 0.02$ Å. When more helium is added, 2D solid helium covers the whole bundle surface. We have now determined the vibrational dynamics of these 1D and 2D solids, the dynamic structure factor, $S(Q,\omega)$. From the inelastic intensity integrated over all $\omega$ we obtain the MS amplitude of vibration along 1D chain ($u_2$) = 0.28 Å$^2$ for Lindemann ratio $\gamma = ((u_2)^2/\langle u_2^2 \rangle/\langle u_2^2 \rangle) = 0.15$ which is less than the bulk solid value near melting. The vibrational density states (DOS) of the 2D solid shows a gap at $\omega = 0.75$ meV indicating a commensurate solid as found for $^3\text{He}$ and $^3\text{He}$ on graphite surfaces. In contrast the 1D DOS shows little or no gap and the DOS goes uniformly to zero as $\omega \rightarrow 0$. [1] Pearce et al. Phys. Rev. Lett. 95, 185302 (2005).

9:00AM P17.00006 100-fold reduction of 2D spin-polarized hydrogen gas’s clock-shifts explained . KADEN R.A. HAZZARD, ERICH J. MUELLER, Cornell University — Recent experiments have observed that when two-dimensional spin-polarized hydrogen is adsorbed on a superfluid helium film, the density dependent shift of the 1S-2S spectral line (clock shift) is 100 times smaller than expected [1]. By studying the theory of interactions between hydrogen atoms and helium films, we show that when helium-mediated hydrogen-hydrogen interactions dramatically reduce the clock shift. The mediated potential is sensitive to experimental parameters, such as temperature and $^3\text{He}$ concentration. This explains another mysterious experimental result: we find that increasing $^3\text{He}$ concentration increases the clock-shift, as observed. In contrast, the naive picture which neglects mediated interactions predicts the clock-shift to decrease with $^3\text{He}$ concentration due to deconfinement of the hydrogen gas. [1] J. Ahokas, J. Järvinen, and S. Vasiliev, Phys. Rev. Lett. 98, 43004 (2007).
9:12AM P17.00007 Bound spin waves in the ferromagnetic layer of $^3$He on highly oriented graphite\textsuperscript{1}, LEI GUO, JINSHAN ZHANG, C.M. GOULD, H.M. BOZLER, Univ. of Southern California — The second monolayer of $^3$He on graphites such as Grafoil becomes highly ordered at millidegree temperatures. This system is a good model for nanoscale two-dimensional magnetism because of the large number of separated two-dimensional planes. Motivated by our interest in increasing the structural coherence of the graphite samples that we study, we have used exfoliated ZYX grade graphite as a substrate for our recent experiments. Much of the general picture of finite temperature ordering with ZYX is similar to Grafoil. However, as a byproduct of our increased structural coherence, we have observed several distinct resonances in the ordered spin system. This result is surprising because the structural size of platelets of graphite is not controlled. Nevertheless, the separation of the resonances is consistent with bound two-dimensional spin waves with length scales consistent with the average sizes of the graphite platelets. We will present our analysis of the temperature dependence of the spin wave modes.

\textsuperscript{1}Supported by NSF.

9:24AM P17.00008 Spin Pumping in Superfluid $^3$He in High Magnetic Field\textsuperscript{1}. H. KOJIMA, Rutgers University, K. SUZUKI, Y. AOKI, A. YAMAGUCHI, H. ISHIMOTO, ISSP. U. of Tokyo — The spin flow dynamics in superfluid $^3$He $A_1$ phase in magnetic field has been studied up to 13 tesla. The apparatus consists of a large reservoir of $A_1$ phase in which a small enclosed chamber with a built-in differential pressure sensor is immersed. The chamber is connected to the reservoir via a superleak channel. The channel is fabricated from Macor parts such that the residual heat leak is much reduced from those in our experiments. Our focus is on the measurement of relaxation of the induced pressure subsequent to either magnetically induced spin-polarized superflow or by electrostatic spin pumping. In general, both methods of measurement show that the relaxation time $\tau$ of the induced pressure tends to vanish smoothly as the transition temperature $T_\lambda$ is approached. However, the observed dependence of $\tau$ on magnetic field is different. The measured $\tau$ by the field gradient method continues to increase up to 8 tesla. On the other hand, $\tau$ measured by the spin pumping method tends to saturate to a constant between 5 and 13 tesla. The discrepancy is unexpected and not yet understood.

\textsuperscript{1}Research supported in part by the U.S. NSF grant DMR-0704120, JSPS and MEXT of Japan.

9:36AM P17.00009 Discovery of a New Excited Pair State in Superfluid $^3$He\textsuperscript{1}, JOHN P. DAVIS, JOHANNES POLLANEN, HYOJUNGSOON CHOI, JAMES A. SAULS, WILLIAM P. HALPERIN, Northwestern University — In superfluid $^3$He, the order parameter collective modes correspond to excited states of the $^3$He Cooper pairs and are classified by their total angular momentum, $J = L + S$. Many of these modes with $J \leq 2$ have been experimentally observed through longitudinal sound measurements or NMR. As a result of coupling to the collective mode with $J = 2$ and $m_J = \pm 1$ there is an enhanced restoring force for transverse sound in pairs. $^3$He-$B$. Previously, we have used the interference of transverse sound waves to study this collective mode. Recently we have discovered a new coupling to transverse sound near the pair-breaking threshold with the classic signatures of a collective mode. Application of a magnetic field results in circular acoustic birefringence and a new acoustic Faraday effect, from which we extract the corresponding Verdet constant. Selection rules for the coupling to transverse sound and acoustic birefringence require this mode to have $J \geq 4$, suggesting that this mode is most likely the $J = 4$ ($m_J = \pm 1$) mode resulting from an attractive $f$-wave pairing interaction in this $p$-wave superfluid.

\textsuperscript{1}We acknowledge support from the NSF. DMR-0703656.

9:48AM P17.00010 Direct Sound Propagation in Superfluid $^3$He-A in 98% Aerogel\textsuperscript{1}, B. H. MOON, N. MASUHARA, P. BHUPATHI, M. GONZALEZ, M. W. MEISEL, Y. LEE, NHMFL and Dept. of Phys. Univ. of Florida, Gainesville, FL 32611, N. MULDERS, Dept. of Phys and Astronomy, University of Delaware, Newark, DE 19716 — Liquid $^3$He impregnated in high porosity aerogel has been studied extensively in recent years since its unique structure provides static impurities in this system. The fragile nature of $p$-wave Cooper pairs against impurity was clearly demonstrated by the significant depression of the superfluid transition. The scattering off the aerogel also significantly modifies the low energy excitation by inducing impurity bound states inside the gap. Recent ultrasound attenuation measurements performed in the $B$-like phase of superfluid $^3$He in 98% porosity aerogel revealed many interesting features and provided strong experimental evidence of gapless superfluidity. We conducted high frequency sound propagation measurements at 6.22 MHz in the $A$-like phase of superfluid $^3$He. The $A$-like phase is stabilized by magnetic fields (up to 4 kG) applied perpendicular to the direction of sound propagation. We present our preliminary results of ultrasound attenuation down to the zero temperature limit at 29 bar and the field dependent A-B transition identified by the jump in attenuation.

\textsuperscript{1}Supported by NSF DMR-0239483 (YL) and DMR-0701400 (MWM).

10:00AM P17.00011 Effect of Global Anisotropy on Superfluid $^3$He in Compressed Aerogels\textsuperscript{1}, P. BHUPATHI, B. H. MOON, M. GONZALEZ, Y. LEE, Department of Physics, University of Florida, Gainesville, FL 32611-8440, N. MULDERS, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 — The importance of anisotropic scattering on the superfluid phases of $^3$He has been addressed recently and experiments using uniaxially distorted aerogel have been proposed in order to elucidate the influence of global anisotropy on the A-B transition\textsuperscript{2}. We performed high frequency transverse acoustic impedance measurements on superfluid $^3$He confined in 98% porosity aerogel at 29 bar. The aerogel cylinder is compressed along the symmetry axis to generate global anisotropy. With 10% axial compression, our measurements reveal that the A-like to B-like transition is absent on cooling down to $\sim 350 \mu K$ in the absence of magnetic field and in magnetic fields up to 3 KG. This behavior is in contrast to that in uncompressed aerogels, in which the supercooled A-like to B-like transitions have been identified by various experimental techniques. Our results are consistent with the theoretical prediction by Aoyama and Ikeda.

\textsuperscript{1}This work is supported by NSF grant no. DMR-0239483 (Y.L).

10:12AM P17.00012 Low field NMR in aerogel-confined superfluid $^3$He\textsuperscript{1}. YULIANG DU, H.M. BOZLER, C.M. GOULD, Univ. of Southern California — The superfluid phases of bulk liquid $^3$He were convincingly identified through their longitudinal and transverse NMR spectra. The order parameters of the superfluid phases of $^3$He confined within aerogel have generally been assumed to be identical to those in bulk liquid. While that identification has not been contradicted by experimental data, it has not yet been tested as carefully as in bulk. Fomin has suggested that the A-like phase in aerogel could be an axiplanar state, distinct from the bulk axial state. We have tested the identification by studying low-field NMR which is more sensitive to the distinction between the candidate states. Using the dc SQUID based NMR detection system developed in our laboratory over many years we have studied both longitudinal and transverse resonance spectra in 99.5% porosity aerogel in magnetic fields of 1-4 mT, an order of magnitude lower than previous NMR work. Our work shows qualitative features similar to those found in higher magnetic fields. While we were unable to resolve the longitudinal resonance, transverse resonance measurements exhibit a characteristic field- and temperature-dependence.

\textsuperscript{1}Supported by the National Science Foundation.
10:24AM P17.00013 Dynamics of Quantum Vortices, LARA THOMPSON, UBC, PHILIP STAMP, UBC, PITT —
Quantized vortices exist in systems ranging from low-T magnets, to superfluids and superconductors; however, their dynamics remain controversial. Even the existence of a force acting transverse to the motion (like a Lorentz force) relative to thermal quasiparticles has been widely debated. Quite remarkably, it remains unresolved just what forces act on a quantum vortex. From an influence functional calculation, we show that the expected log divergent mass generalizes to a frequency dependent mass and damping, which, in time, manifest as memory dependent damping forces, acting both longitudinal and transverse to current motion. Based on our numerical simulations to directly estimate this force, we predict the existence of new, previously unconsidered unsuppressed quantum vortices within disc and insulating magnets, we are able to find the various forces, including those resulting from vortex-magnon interactions, and derive their dynamics. In contrast to superfluids and superconductors, an experimental test in insulating magnets should be possible using existing methods.

Wednesday, March 12, 2008 8:00AM - 11:00AM —
Session P18 DPOLY: Polymer Nanocomposites — Morial Convention Center 210

8:00AM P18.00001 Disordered nanoparticle interfaces for defect-tolerance in the self-assembly of block-copolymers, KEVIN YAGER, ALAMGIR KARIM, Polymers Division, National Institute of Standards and Technology, ERIC AMIS, Materials Science and Engineering Laboratory, National Institute of Standards and Technology — Directed self-assembly is a promising route to controlling the nanostructure and surface properties of coatings. We describe a general and robust strategy for controlling the self-assembly of thin films by tuning the film-substrate interaction, using an inherently defective nanoparticle layer. These tunable surfaces exhibit hierarchical and controllable roughness via spin-coating conditions (20 nm silica nanoparticle solutions), and tunable surface energy via selective oxidation. Independent manipulation of these parameters enables control of self-assembled order for coatings cast on these tunable substrates. In particular, we demonstrate control of the orientation of lamellae in poly(3,4-dianilinestyrene-block-methyl methacrylate), with expression of the vertical lamellae orientation under certain conditions. Moreover we demonstrate that the lamellae orientation depends upon film thickness in a periodic manner in the range from 30 nm to 240 nm, which provides insights into the fundamental driving forces in this self-assembly. The proposed assembly orientations are compared with theory and validated by complementary neutron reflectivity and small-angle neutron scattering measurements.

8:12AM P18.00002 Anisotropic Self-Assembly of Spherical Nanoparticles in Polymer Composites, PINAR AKCORA, SANAT K. KUMAR, Columbia University, YU LI, BRIAN BENICEWICZ, LINDA S. SCHADLER, Rensselaer Polytechnic Institute, DEVIRM ACEHAN, New York University, JACK F. DOUGLAS, National Institute of Standard and Technology, COLUMBIA UNIVERSITY COLLABORATION, RPI COLLABORATION, NYU COLLABORATION, NIST COLLABORATION — I will present our recent experimental findings on the organization of isotropic polymer grafted particles forming anisotropic three dimensional structures. Earlier studies have shown that particle shape and anisotropic particle interactions determine the self-assembly process. It has been also shown that isotropic particles can form string like colloidal assemblies within monolayers at two-dimensions but at high particle loadings. Here, I will present the three dimensional sheet structures formed by mixing spherical nanoparticles that are grafted uniformly with long polymers and dispersed in the same homopolymer matrices at relatively low loadings. The molecular origin of this anisotropic organization is the combined short ranged repulsive forces and longer ranged attraction interaction between the particles that is also supported through theory and numerical simulations. The self-assembly of isotropic nanoparticles into anisotropic structures within polymer melts has profound application potentials in improving the electrical and mechanical properties of composite materials.

8:24AM P18.00003 Enthalpic Relaxation of Silica-Polyvinyl Acetate Nanocomposites, SAMUEL AMANUEL, Department of Physics and Astronomy, Union College, Schenectady, NY 12308, SANFORD STEINSTEIN, Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180 — While the effects of nanoparticle size and surface treatment on the glass transition temperature have received well-deserved attention, their effects on other physical parameters associated with the glass transition have received less interest. In order to understand how the incorporation of nanoparticles affects the enthalpic relaxations associated with the glass transition, Differential Scanning Calorimeter (DSC) measurements were carried out on silica-polyvinyl acetate nanocomposites with respect to filler content, annealing temperature and annealing period. As expected, longer annealing periods below the glass transition temperature result in an increase of the subsequent enthalpic relaxations. However, the presence of filler substantially reduces the enthalpic relaxation relative to that of the neat polymer. Even after corrections to account for filler weight, the enthalpic relaxations still decrease monotonically with increasing filler content. The underlying enthalpic relaxations and the effects suppressed by the fillers are specific to the annealing temperature. These results suggest a significant alteration of the physical state of the matrix material by the presence of the filler particles.

8:36AM P18.00004 Particle structuring in stretched soft/hard nanocomposite, YANN LE DIAGON, UPME, STEPHANIE MALLARINO, CHRISTIAN FREITIGNY, CNRS, PPMD TEAM — The deformation mechanisms of nanocomposites made of disordered rigid inclusions imbedded in a soft matrix are rather complex as the local geometry and mechanical responses are very intricate. Atomic force microscopy (AFM) is used to analyze the surface of a model elastomer submitted to uniaxial traction. Since the sample contains monodisperse spherical rigid inclusions, images easily yield statistical data on the positions of the fillers. As expected, it is observed that the displacement field is affine at large scales. At short range, important deviations are observed. Two factors present the characteristic “butterfly” patterns, similar to the neutron scattering patterns obtained on many deformed heterogeneous materials. We show that mechanical confinement of the inter-particular matrix regions must be taken into account in order to explain the results. Finally AFM images reveal higher order correlations: Fillers are observed to be arranged along lines which are roughly perpendicular to the stretching direction. Such a characteristic organization seems to be characteristic of the soft/hard disordered systems.

8:48AM P18.00005 Particle inclusion effect on the rheological properties of polymeric materials, GREGORY TOEPPEPERWEIN, GEORGE PAPAKONSTANTOPOULOS, JUAN DE PABLO, University of Wisconsin — Recently developed algorithms have permitted the extraction of the primitive path and the entanglement length, Ne, from simulations of polymer melts. Experimental studies on the effect of the addition of nanoparticles to a polymer melt have revealed that nanoparticles can alter the plateau modulus and subsequently the entanglement length of the polymer. We use simulations to directly estimate the entanglement length of nanocomposite systems to study the effect of spherical and anisotropic nanoparticles on the entanglement length of a polymer matrix. In this work we present a systematic study of the effects of particle-particle interactions, particle size, aspect ratio and volume fraction. Advanced Monte Carlo techniques involving chain connectivity algorithms are used to create statistically independent configurations. Attractive, neutral and repulsive polymer particle interaction are considered. Furthermore, we examine the effect of different assumptions on the calculation of Ne.

9:00AM P18.00006 Dimensional Analysis of Percolation Theory: Applications to Polymer Composites, DERRICK STEVENS, Dept. of Physics, North Carolina State University (NCSU), TORISSA HOFFMAN, Dept. of Physics, NCSU, RUSSELL GORGA, Dept. of Textiles Engineering, Chemistry and Science, NCSU, LAURA CLARK, Dept. of Physics, NCSU — Percolation theory is well known to describe functional phenomena in polymer composites such as electrical conductivity, when combining a conducting particle and insulating matrix. Nanostructured composites can, however, present unique morphologies that are not easily described by the typical one, two, or three-dimensional viewpoint. One example is random mats of polymer/carbon nanotube (or silver nanoparticle) composite nanofibers. With this motivation, Monte Carlo simulations were developed to investigate various effects within such a fibrous geometry, including changes to the critical volume fraction due to the dimensionality: particle aspect ratio, relative size of particle and fiber (or film), sample size, continuous vs. porous structure. From these simulations a model was developed to predict the percolation threshold based on the dimensionality of the system. The results of these simulations and the derived model will be presented.
A hybrid particle-field (HPF) simulation method for polymer-nanoparticle composites, DOMINIK DUECHS, UC Santa Barbara, SCOTT SIDES, Tech-X Corp., GLENN FREDRICKSON, UC Santa Barbara — A hybrid particle-field (HPF) simulation method for composite systems of polymers and sets of movable particles is presented. The particles are implemented as cavities in an otherwise flat density profile of the polymeric background (corresponding to overall incompressibility), enabling a common treatment of both components in the general framework of well-known self-consistent field theory (SCFT). The particle movements are controlled by force-biased and, where applicable, torque-biased propagation schemes. Particles and polymers interact via local contact interactions originating at the particle surfaces. Simulations with orientationally homogeneous spheres as well as with spheres possessing two distinct sets of interaction parameters on their two hemispheres are compared to experimental results.

Responsive Assemblies: Gold Nanoparticles with Mixed Ligands in Microphase Separated Block Copolymers, JINBO HE, ELIZABETH GLOGOWSKI, QIFANG LI, TODD EMRICK, THOMAS RUSSELL, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, XUEFA LI, JIN WANG, Advanced Photon Source, Argonne National Laboratory, Argonne — A simple method for controlling the spatial distribution of gold nanoparticles in a polystyrene-block-poly (2-vinylpyridine) (PS-b-P2VP) diblock copolymer is shown. By varying the ligand functionality of the gold nanoparticles, as well as the processing and annealing conditions, the distribution of gold nanoparticles in the microdomains of the diblock copolymer was controlled and altered. In addition, the presence of nanoparticles was also found to affect the diblock copolymer morphology. Subsequent thermal annealing causes a coarsening of the nanoparticles, and a sequestration of the nanoparticles to the P2VP microdomain. Further heating leads to an expulsion of the particles from the microdomains, a modification of the interfacial interactions, and a reorientation of the copolymer morphology.

Physical Characterization of Hierarchically Structured Nanocomposites, ROSS BEHLING, ERIC COCHRAN, Iowa State University — In this contribution we present various aspects of the thermodynamics of self assembly in block copolymer / layered silicate nanocomposites (BCLPLs). Hierarchically structured BCLPLs were prepared using an in situ atom transfer radical polymerization (ATRP) approach. The three part synthesis of the materials included an ion exchange functionalization of the clays, sonication during styrene (St) polymerization, and 103˚C for the St. This is a significant Tg enhancement for atactic tBA (Tg = 42˚C) and is attributed to the chain extension which occurs in the confined microscopy (SEM) and transmission electron microscopy (TEM).
Using x-ray photon correlation spectroscopy, we have studied slow, wave vector and temperature dependent microrheology of nano particles embedded in a soft glassy matrix with unique viscoelastic properties. The measurements were done for a polymer matrix (PMMA) using gold nanoparticles as probe. The intensity autocorrelation function exhibits a cross-over from compressed to stretched relaxation behavior on cooling from above the glass transition temperature ($T_g$) of PMMA. Although stretched exponential relaxation is expected in the glassy state one would expect simple exponential relaxation above the $T_g$. We also find that the relaxation time ($\tau_g$) of PMMA follows $\tau \sim q^{-1}$ dependence indicating super-diffusive motion of nanoparticles. Interestingly, we have also observed subtle effects like length scale dependence of the stretching exponent. This points to the importance of the nanoparticles in modifying the viscoelastic property of the polymer matrix and highlights the strength of this technique in extracting their micro-rheological properties.

Wednesday, March 12, 2008 8:00AM - 11:00AM
Session P20 DMP: Focus Session: Engineering Interfaces for New Materials I: Internal Interfaces
Morial Convention Center 212

8:00AM P20.00001 Segregation Effects at Internal Interfaces in Alloys: Atom-Probe Tomographic Experiments and Simulations
DAVID SEIDMAN, Northwestern University — This talk first focuses on experimental studies of solute segregation effects on an atomic scale of solute segregation at grain boundaries (GBs) and heterophase interfaces employing atom-probe field-ion microscopy and three-dimensional atom-probe tomography; both instruments provide a spatial resolution of ca. 0.2 nm in direct space. It is demonstrated that the Gibbsian interfacial excess of solute at an internal interface depends on its five macroscopic degrees of freedom (DOFs), which is consistent with J. Cahn’s local phase rules for GBs and heterophase interfaces. Experimental data is presented for GBs in metallic alloys (e.g. Fe-Si, Al-Sc-Mg, Ni-Al-Cr alloys), and metal silicide/silicon and indium arsenide heterophase interfaces. Secondly, atomic-scale simulations will be presented of GB segregation in binary metallic alloys described by embedded-atom method potentials employing Metropolis algorithm Monte Carlo simulations, which further demonstrate the intimate relationships between GB structure, on an atomic scale, and the Gibbsian interfacial excess of solute. It is also shown how the microscopic DOFs of a GB affect the Gibbsian interfacial excess of solute. Additionally, the results of atom-probe tomographic studies of segregation effects at heterophase interfaces between the gamma (f.c.c.) and gamma prime (L1_2) structure heterophase interfaces in Ni-Al-Cr alloys are discussed and compared in detail with the results of lattice kinetic Monte Carlo (LKMC) simulations, which involves a vacancy mediated diffusion mechanism. The LKMC simulation allow us to explain the role of vacancy-solute binding energies on the observed concentration profiles of Ni, Al, and Cr between the gamma and gamma prime phases. These detailed experimental and simulation studies of segregation effects result in a relatively new atomistic picture of segregation at internal interfaces that differs from the conventional wisdoms found in the literature concerning segregation.

8:36AM P20.00002 Interface structure and radiation damage resistance in Cu-Nb multilayer nanocomposites
MICHAEL DEMKOWICZ, RICHARD HOAGLAND, JOHN HIRTH, Los Alamos National Laboratory — We use atomistic simulations to show that misfit dislocations in Cu-Nb interfaces can shift location between two adjacent planes by forming pairs of extended jogs, a mechanism that involves removal or insertion of atoms. Different jog combinations give rise to interface structures with unlike densities but nearly degenerate energies, making Cu-Nb interfaces virtually inexhaustible sinks for irradiation-induced point defects and catalysts for efficient Frankel pair recombination.

8:48AM P20.00003 Threshold Shear Stresses at Aluminum-Silicon interfaces
ALICE NOREYAN, University of Windsor. YUE QI, General Motors, VESSELIN STOILOV, University of Windsor — The critical shear stress at Cu-Nb interfaces can shift location between two adjacent planes by forming pairs of extended jogs, a mechanism that involves removal or insertion of atoms. Different jog combinations give rise to interface structures with unlike densities but nearly degenerate energies, making Cu-Nb interfaces virtually inexhaustible sinks for irradiation-induced point defects and catalysts for efficient Frankel pair recombination.

9:00AM P20.00004 The strength characterization of Al/Si interfaces with a hybrid nanoindentation/FEM method
SHUMAN XIA, Division of Engineering, Brown University. YUE QI, THOMAS A. PERRY, GM Research & Development Center, KYUNG-SUK KIM, Division of Engineering, Brown University — The mechanical property characterization of the reinforcement/matrix interface in a metal matrix composite (MMC) is entailed for tailoring the interface in the microstructure design of the composite. In this work we developed a hybrid method to characterize the interface strength of an MMC, combining a nanoindentation experiment and a finite element analysis. The nanoindentation experiment was carried out by indenting individual reinforcement particles on a free surface with a nanoindenter. The dependence of indentation response on the interface properties was systematically studied through the finite element analysis with cohesive zone modeling of the interface failure. The interface strength could then be extracted from the comparison between the experimental and FEM results. With this method, the shear strength of an Al/Si interface was measured approximately 240MPa which compares well with the lower bound of an atomistic simulation with a modified EAM potential. The intrinsic fracture toughness of the interface crack tip surrounded by densely populated dislocations was measured 0.25 J/m2. We also studied the effect of the strontium modification on the interface strength with this hybrid method.

* 1 NSF, DOE, ONR
* 2 This work was supported by the Los Alamos National Laboratory Directed Research and Development Program (LDRD) and the Los Alamos National Laboratory Directors Fellowship Program.
* 3 This work was supported by National Science and Research Engineering Council of Canada and General Motors Canada under CRD 36799
9:12AM P20.00005 Atomic Resolution Study of the Interfacial Bonding at Si₃N₄/CeO₂₋δ Grain Boundaries¹. ROBERT F. KLIE, WERONIKA WALKOSZ, SERDAR OGUT, University of Illinois at Chicago, A. BORISEVICH, PAUL F. BECHER, STEVE J. PENNYCOOK, JUAN C. IDROBO, Materials Science and Technology Division, Oak Ridge National Laboratory — Using a combination of atomic resolution Z-contrast imaging and electron energy-loss spectroscopy (EELS) in the scanning transmission electron microscope, we examine the atomic and electronic structures at the interface between Si₃N₄ (10T0) and CeO₂₋δ inter-granular film (IGF). Ce atoms are observed to segregate to the interface in a two-layer periodic arrangement, which is significantly different compared to the structure observed in a previous study. Our EELS experiments show that (i) oxygen is present at the interface in direct contact with the terminating Si₃N₄ open-ring structures, (ii) the Ce valence state changes from +3 to +4 in going from the interface into the IGF, and (iii) while the N concentration decreases away from the Si₃N₄ grains into the IGF, the Si concentration remains uniform across the whole width of the IGF. Possible reasons for these observed structural and electronic variations at the interface and their implications for future studies on Si₃N₄/rare-earth oxide interfaces are briefly discussed.

9:24AM P20.00006 The Influences of different cathode materials on Tris-(8-Hydroxyquinoline)- Aluminum Doped with CsNO₃ in Organic Light emitting Devices. MEI-HSIN CHEN, YIN-JULI LU, CHUNG-CHIH WU, CHIH-I WU, Graduate Institute of Photonics and Optoelectronics — This paper presents the investigations of interfacial interactions and electron-injection mechanisms between cesium nitrate (CsNO₃) and different cathode materials. By using ultraviolet and x-ray photoemission spectroscopy, the properties of electronic structures and the interfacial chemistry are studied. According to our results, there exists a phenomenon of electron exchange at the interface results in changes of Aluminum 2s core level binding energy by 1 eV when aluminum was deposited on CsNO₃. This means electrons transfer from cathode materials to the surface of CsNO₃, forming a strong dipolar field at the interface and reduction of the electron injection barrier. But, in contract, there exists nearly no reaction between CsNO₃ and silver cathode. The evidences show that CsNO₃ is more effective only with aluminum cathode due to a reaction between Aluminum, Cesium and Nitrogen atoms.

9:36AM P20.00007 Atomic-resolution study of cobalt valence and spin-state transitions in Ca₃Co₄O₉ using in-situ scanning transmission electron microscopy. GUANG YANG, YUAN ZHAO, ROBERT KLIE, Department of Physics, University of Illinois at Chicago — The misfit-layered Ca₃Co₄O₉ (CCO) has been of great interest due to its high thermo-electric power and thermal stability. The CCO structure consists of five layers: three rock salt-type layers Ca₃Co₂O₆ are sandwiched between two CdI₂-type Co₂O₆ layers along the c-direction. The presence of different Co valence states is assumed to account for the thermal stability of CCO, and the abrupt changes of electrical resistivity at 420K is believed to be due to a Co spin-state transition. Here, we combine scanning transmission electron microscopy (STEM) with electron energy loss spectroscopy (EELS) to study the atomic and electronic structure of CCO. Using atomic-column resolved EELS, the Co valence states in the different layers are quantified and significant charge transfer from CoO₆ to Ca₂Co₂O₆ is measured. The effects of the potential spin-state transition at 420K on the local structure will be studied by in-situ heating experiments. We will show how atomic-resolution Z-contrast imaging in combination with EELS and in-situ experiments can be utilized to understand the effects of interfacial charge transfer and spin-state transitions in complex oxide materials.

9:48AM P20.00008 The Classical Size Effect: Impact of Grain Boundaries on Resistivity in Encapsulated Cu Thin Films¹. TIK SUN, BO YAO, ANDREW WARREN, KEVIN COFFEY, University of Central Florida, VINEET KUMAR, KATAYUN BARMAK, Carnegie Mellon University — Surface and grain boundary electron scattering contribute significantly to resistivity as the dimensions of polycrystalline metallic conductors are reduced to, and below, the electron mean free path. A methodology is developed to independently evaluate surface and grain boundary scattering in encapsulated polycrystalline Cu thin films, with thicknesses in the range of 27-165 nm. The film resistivity, measured at both room temperature and at 4K, is compared for samples having different grain sizes (as determined from 400 to 1,500 grains per sample) and film thicknesses. The experimental data is compared to models of surface and grain boundary scattering in thin films. The resistivity contribution from grain boundary scattering is found to be significantly greater than that of surface scattering in Cu thin films which allows a quantitative measurement of the parameters for the Mayadas-Shatzkes model. It is also found that the Ta barrier layer prohibits grain growth which explains the higher resistivities observed in encapsulated Cu samples with Ta barrier layers.

¹This research is supported by the SRC, Task 1292-008 and the MRSEC under NSF DMR-0520425.

10:00AM P20.00009 Resistivity induced by electron-grain boundary scattering on thin gold films deposited on mica substrates under high vacuum. RAUL C. MUNOZ, RICARDO HENRIQUEZ, PABLO LEIVA, SIMON OYARZUN, MARCO A. SUAREZ, PAULA MANRIQUE, SIMON SILVA, GERMAN KREMER, LUIS MORAGA, Department of Physics, University of Chile — We report measurements of the room temperature resistivity and of the grain size distribution on a family of gold films deposited onto mica substrates under high vacuum. The films are of approximately the same thickness (100 nm ± 10%), deposited at the same rate (3 nm/min), varying both the temperature of the substrate and the annealing temperature (if any) between −170 °C and +270 °C. The grain distribution was measured with a Scanning Tunneling Microscope. The average grain size decreases from approximately 200 nm to a few nm, when the temperature of the substrate decreases from +270 °C to −170 °C during evaporation. The monotonic decrease in grain size leads to a monotonic increase in resistivity of almost one order of magnitude. The resistivity of the film evaporated with the substrate held at +270 °C and annealed for one hour at +270 °C after evaporation, exhibits a room temperature resistivity only a few percent larger than crystalline gold. Research funded by FONDECYT 1040723.

10:12AM P20.00010 The effect of hydrogen content on intrinsic stress in nanocrystalline diamond (NCD) coatings. HAI BO GUO, University of South Carolina, YUE QI, XINGCHENG XIAO, General Motors R&D, ABHISHEK KOTHARI, BRIAN W. SHELDON, Brown University, MATERIALS AND PROCESSES LAB, GENERAL MOTORS R&D & COLLABORATION, UNIVERSITY OF SOUTH CAROLINA COLLABORATION, BROWN UNIVERSITY COLLABORATION — The stress control is critical to ensure the reliability of nanocrystalline diamond (NCD) coatings. We found the intrinsic stress in NCD is tensile at deposition temperature above 700°C. Decreasing the deposition temperature decreases this tensile stress, and eventually leads to compressive stresses. The stress evolution appears to be largely dictated by grain boundary formation and hydrogen incorporation, which involves absorption, desorption, and recombination kinetics on diamond surfaces. The competition between these reactions indicates that the hydrogen coverage at interfaces should increase with decreasing growth temperature. This is consistent with Raman spectra and elastic recoil detection. To understand hydrogen effects, density functional theory (DFT) is used to model the coalescence of two diamond grains that approach each other to form a grain boundary. The two surfaces exhibit attractive forces when hydrogen coverage is less than 75%, and repulsive forces when all the surface bonds are hydrogen terminated (100% hydrogen coverage). In this way, differences in the hydrogen coverage can explain the observed transition from tensile to compressive intrinsic stress as the growth temperature decreases.
10:24AM P20.00011 Super Hard Cubic Phases of Period VI Transition Metal Nitrides: A First Principles Investigation 1, S.V. KHARE, Department of Physics, University of Toledo, S.K.R. PATIL, Department of MIME, University of Toledo, N.M. MANGALE, Department of EECS, University of Toledo, S. MARSILLAC, Department of Physics, University of Toledo — We report a systematic study of mechanical and electronic properties of 32 cubic phases of nitrides of the transition metals M (M = Hf, Ta, W, Re, Os, Ir, Pt, Au), in zinc-blende, rocksalt, pyrite, and fluorite structure using ab initio computations. Our results reveal that MN2 (M = W, Re, Os, Ir, Pt, Au) in pyrite phase, have a bulk moduli greater than 330 GPa, MN2 (M = Re, Os, Ir) in fluorite phase have a bulk moduli greater than 350 GPa and TaN in rocksalt phase has a bulk modulus of 380 GPa making them candidates for super hard materials. Based on the bulk and shear modulus for stable phases, potential hard coating materials for cutting tools have been identified. Structural stability of stable binding phases has been obtained by linked to a transition chain. The high values of bulk moduli are attributed to strong bonding of transition metal d-orbitals with nitrogen p-orbitals. The trend in the bulk modulus is related to the valence electron density of these materials.

1We thank Wright Patterson Air Force Base and Ohio Board of Regents for supporting this work.

10:36AM P20.00012 Coherent atomic motion in nano-crystal film 1, JUNJIE LI, XUAN WANG, SHOUHUA NIE, RICHARD CLINITE, JIANMING CAO, Physics Department and National High Magnetic Field Laboratory, Florida State University — We report a theoretical study of the structural dynamics in metallic film in response to ultrafast laser heating. A two-dimensional model using a harmonic approximation is used to simulate the lattice dynamics. We examine the response of the adatom. The linear arrangement of favorable binding sites induces the self-organization of Au atoms into chains. For every ad-chain, the number of neighbors is increased by 1 and the distance between neighboring adatoms is increased by a constant value. The adatom-atom interaction in a metal film is considered in order to determine the modes of lattice motions. Moreover, a large projection of coherent lattice oscillation in the in-plane direction is found, which was previously thought to be very small and was neglected in one-dimensional models. The simulation agrees well with our femtosecond electron diffraction measurements.

1Physics Department and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310

10:48AM P20.00013 Tuning physical properties by assembling subnanometer inorganic and organic units, YONG ZHANG, P.A. PARILLA, S.P. AHRENKIEL, A. MASCARENHAS, NREL, Z. ISLAM, Y. REN, P.L. LEE, APS/ANL, M.J. MCNEVIN, UC. Boulder, I. NAUMOV, H.X. FU, U. Arkansas, X.Y. HUANG, J. LI, Rutgers U. — Designing inorganic-organic hybrid materials in a nanoscopic scale allows taking the full advantage of the two worlds, which has recently been demonstrated in a new family of hybrid crystalline materials that are the fully ordered assemblies of sub-nanometer scale inorganic units (e.g., few monolayer-thick slab, single atomic chain) and organic molecules[1]. They have been shown to exhibit a number of unique properties that are not readily available in either of the components or their nanostructures: for instance, strongly enhanced exciton-polariton absorption and exciton binding energy[2], a massive bandgap blue shift (~2 eV) from that of the bulk inorganic semiconductor[3], and fine-tuning of thermal expansion and achieving zero-thermal-expansion[4]. They have great potential for applications in areas including transparent conductors, thermoelectric materials, UV optoelectronic devices, because of their unusual electronic, vibrational and optical properties and the flexibility in tailoring the material properties adapting to the specific application requirements. [1] X. H. Huang et al., JACS 125, 7049 (03). [2] Y. Zhang et al., PRL 96, 26405 (06). [3] B. Fluegel et al., PRB 70, 205308 (04). [4] Y. Zhang et al., PRL 99, 215901 (07).

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P21 DCP: Focus Session: Fundamental Issues in Catalysis | Morial Convention Center 213

8:00AM P21.00001 The role of hot electrons in catalysis science, GABOR A. SOMORJAI, Department of Chemistry, University of California Berkeley — One long-standing observation in the field of heterogeneous catalysis is that the activity and selectivity in certain reactions is dramatically affected by the oxide onto which the metal nanoparticles are deposited, even though the oxide itself is not active in catalysis. Recently, studies which detected hot electron formation at metal surfaces helped to explain these curious findings. Pulse probe experiments have detected hot electron formation within femtoseconds when photons are incident on a metal surface. Experiments indicate that the mean free path of these hot electrons is on the order of 5 nm, which is in the range of the size of catalytic nanoparticles. Further studies indicate that exothermic catalytic reactions can also produce hot electrons readily, for example CO oxidation or the reaction of hydrogen and oxygen to form water. We have constructed a “catalytic nanodiode” in our laboratory whereby we carry out catalytic reactions at high and continuous turnover and, using a Schottky barrier, collect hot electrons. Simultaneous measurement of turnover frequency and hot electron current during CO oxidation has shown that the hot electron current and the turnover rate for the reaction are correlated. This implies that the catalytic activity at the oxide-metal interface in certain catalytic reactions is associated with the hot electron flow.

8:36AM P21.00002 CO oxidation over noble metals: The continuum from ultrahigh vacuum to atmospheric pressures, DAVID GOODMAN, Texas A&M University — Catalytic oxidation of CO has been investigated for many decades by numerous researchers and is considered to be one of the best understood catalytic reactions. Because of its importance in pollution control, fuel cells, etc., this reaction has received considerable attention for fundamental and practical reasons. Removal of CO from automobile exhaust is accomplished by catalytic converters using supported Pt-group metals of Pt, Pd and Rh catalysts. The catalytically removal of traces of CO from H2 by Pt-group metals to the few ppm level is required for efficient operation in fuel cells. Efforts in our laboratory have addressed the adsorption of CO and the kinetics of CO-oxidation on single crystals and supported metal catalysts over a wide temperature (400–650 K) and pressure (1–10 bar) range. Two active phases, CO-dominated and O-dominated, have been identified for which the mechanisms for CO catalytic oxidation are entirely different. The highly active phase formed in oxygen-rich crystals and supported metal catalysts over a wide temperature (400–650 K) and pressure (1–10 bar) range. Two active phases, CO-dominated and O-dominated, have been identified for which the mechanisms for CO catalytic oxidation are entirely different. The highly active phase formed in oxygen-rich crystals and supported metal catalysts over a wide temperature (400–650 K) and pressure (1–10 bar) range. Two active phases, CO-dominated and O-dominated, have been identified for which the mechanisms for CO catalytic oxidation are entirely different. The highly active phase formed in oxygen-rich.

9:12AM P21.00003 Gold atoms, chains and islands on oxide films: looking at orbitals and counting electrons, HAJO FREUND, Fritz Haber Institute of the Max Planck Society — Low-temperature STM measurements combined with DFT calculations are employed to analyze the adsorption of gold on alumina/NiAl(110). The binding of Au monomers involves breaking of an oxide Al-O bond below the adatom and stabilizing the hence under-coordinated O ion by forming a new bond to an Al atom in the NiAl. The adsorption implies negative charging of the adatom. The linear arrangement of favorable binding sites induces the self-organization of Au atoms into chains. For every ad-chain, the number of electrons, in particular of transfer-electrons from the support, is determined by analyzing the node structure of its HOMO.

9:48AM P21.00004 Theoretical Insights into C1 Surface Chemistry, MATTHEW NEUROCK, University of Virginia — Reforming and partial oxidation of methane as well as other C1 fuels are important processes in the production of hydrogen and synthesis gas and will likely play important roles future energy strategies. Herein we use theory and simulation to examine the reactivity of methane, methanol and dimethylether with CO2, H2O, or O2 supported transition metals. We systematically probe the elementary C-H bond activation as well as the oxidation pathways involved in both reforming as the oxidation of methane and other C1 intermediates over well defined transition metal surfaces, metal alloys and metal nanoparticles. The calculations demonstrate well-established trends in C-H bond activation as the result of changes in the metal, the activating molecule (methane, methanol, and DME) as well as the reaction conditions. The reaction conditions ultimately dictate the surface coverage of carbon and oxygen which have important consequences on the surface reactivity. The theoretical and simulation results are compared with well defined experiments carried out at Berkeley over supported particles.
10:24AM P21.00005 Atomic ordering periodicity and catalytic properties of nanoparticles. VALERI PETKOV, Central Michigan University — Often nanosized particles of crystals are catalytically very active while the corresponding crystals are not. A typical example is gold. The enhanced catalytic performance of nanosized particles, however, does not come merely from their greatly enhanced surface-to-volume ratio. We would like to draw attention to the often overlooked fact that nanosized particles of crystals do not necessarily possess the periodic 3D structure of their bulk counterparts, and this too may impact their catalytic properties substantially. In particular, nanoparticles that do not have a periodic 3D structure may not contain in a well-defined, faceted shape, i.e. may be not terminated by well-defined (usually high energy) atomic planes, as crystalline objects of the same size would be. Hence, nanoparticles may be catalytically more (or less) active than “nanized” crystals. Results from recent structure studies (synchrotron XRD and computer simulations) on 1 – 5 nm Ru, Au and Pt particles will be presented as evidence.

10:36AM P21.00006 First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. SIMONE PICCININ, CATHERINE STAMPFL, The School of Physics, The University of Sydney, Australia, MATTHIAS SCHAFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany — By means of density-functional theory, together with concepts from atomistic thermodynamics, we present a theoretical procedure for describing the structure and stoichiometry of a binary alloy in contact with a surrounding gas phase environment. We apply the approach to the Ag-Cu alloy in an oxygen atmosphere, for which recent results report a superior selectivity for ethylene epoxidation compared to pure silver, the predominant catalyst for this reaction. We first show that the presence of oxygen leads to copper segregation to the surface. Then, considering the surface free energy as a function of the surface Cu composition, we construct the “convex hull”. By including the dependence of the surface free energy of the oxygen chemical potential, we determine the phase diagram of the alloy as a function of temperature, pressure, and Cu surface content. We predict that for conditions typical of the epoxidation reaction, a number of structures can be present on the surface of the alloy including the clean silver surface, thin copper-oxide-like structures, and thick copper oxides. These findings are consistent with, and help explain the recent experimental results. We envisage this approach will be useful and generally applicable for the study of other alloys in contact with a gas or liquid phase.

10:48AM P21.00007 The Cu/ZnO(0001) Surface under Oxidative and Reducing Conditions: A First-principles Study. KAWATU CHUAISIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, School of Physics, BERNARD DELLEY, Paul Scherrer Institut, Villigen Switzerland, CATHERINE STAMPFL, University of Sydney, School of Physics — The Cu/ZnO(0001) surface is widely used as a catalyst for the production of H₂-gas from methanol and is thus of considerable relevance to the emergent hydrogen economy. A key to the further development of this catalyst system is the understanding of the relation between surface structure and function versus environmental conditions such as copper content and state of surface oxidation. Towards this goal, we use density functional theory within the framework of ab initio atomistic thermodynamics to conduct a detailed study of conceivable surface structures under variety of Cu exposures. This produces a surface phase diagram that reveals several distinct regimes of surface reconstruction under oxygen-rich and poor conditions. We correlate our findings with experimental studies, including recent scanning tunneling microscopy results by Dulub et al [1].

References:

Wednesday, March 12, 2008 8:00AM - 10:48AM
Session P22 DMP DPOLY: Focus Session: Organic Electronics: FETs II Morial Convention Center

8:00AM P22.00001 High Performance Solution Processable TFTs. DAVID GUNDLACH, NIST — Organic-based electronic devices offer the potential to significantly impact the functionality and pervasiveness of large-area electronics. We report on soluble acene-based organic thin film transistors (OTFTs) where the microstructure of as-cast films can be precisely controlled via interfacial chemistry. Chemically tailoring the source/drain contact interface is a novel route to self-patterning of soluble small molecule organic semiconductors and enables the growth of highly ordered regions along opposing contact edges which extend into the transistor channel. The unique film forming properties of soluble fluorinated anthradithiophenes allows us to fabricate high performance OTFTs, OTFT circuits, and to deterministically study the influence of the film microstructure on the electrical characteristics of devices. Most recently we have grown single crystals of soluble fluorinated anthradithiophenes by vapor transport method allowing us to probe deeper into their intrinsic properties and determine the potential and limitations of this promising family of oligomers for use in organic-based electronic devices. Co-Authors: O. D. Jurczak¹,², B. H. Hamadani¹, S. K. Park¹, D. A. Mourey⁴, S. Subbianan², A. J. Mood³, R. J. Kline¹, L. C. Tsague², J. G. Kushmerick¹, L. J. Richter², T. N. Jackson¹, and J. E. Anthony³ ¹Semiocductor Electronics Division, ²Surface and Microanalysis Science Division, ³Polymers Division, National Institute of Standards and Technology, Gaithersburg, MD 20899 ⁴Department of Electrical Engineering, The Pennsylvania State University, University Park, PA 16802 ⁵Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055

8:36AM P22.00002 Solution-Processible Thin Film Transistors Using Surface-modified BaTiO³/Polymer Nanocomposites as Gate Insulators. PHILSEOK KIM, Georgia Institute of Technology, XIAOHONG ZHANG, PETER HOTCHKISS, BENOIT DOMERQ, SIMON JONES, SETH MARDER, BERNARD KIPPELEN, JOSEPH PERRY — Polymer/ceramic nanocomposites (NC) can exhibit high k and easily processible materials suitable for gate insulators in organic field-effect transistors (OFET). To obtain high k NCs, high volume fractions (>30 %) of dielectric nanoparticles (NP) are needed. However, due to NP agglomeration at such high volume fractions, poor quality films with high leakage current are obtained. Recently, we have reported that phosphonic acids can strongly bind to BaTiO₃ (BT) NPs and provide enhanced dispersability of NPs in polymer hosts allowing increased volume loading. We report the use of phosphonic acid-modified BT NPs (30–50 nm in poly(4- vinyl phenol) (PVP, k = 3.9) as gate insulators in OFET, which can be readily processed to high quality thin films by simple solution techniques. BT NPs modified with a phosphonic acid bearing a hydrophilic group afforded high quality NC thin films at high loading (up to 75 wt. %) in PVP. Bottom-gate pentacene OFET devices were fabricated on the NC gate insulators. The improved film quality and increased capacitance density (~50 nF/cm², k ~14) were reflected in a low threshold voltage (~1.1 V), a high on/off ratio (~2×10⁶) and ~10⁵ fold decrease in leakage current as compared to that of unmodified BT.

8:48AM P22.00003 Evolution of the Unoccupied States in Alikali metal doped Copper-Phthalocyanine. HUANJUN DING, KIWAN PARK, YONGLI GAO, University of Rochester — The evolution of both the occupied and unoccupied states for Cs and Na-doped Copper-Phthalocyanine (CuPc) has been investigated with photoemission and inverse photoemission spectroscopy (IPES). From the IPES measurement, it is observed that, as the alkali doping ratio increases, the lowest unoccupied molecular orbital (LUMO) of CuPc shifts toward the Fermi level, and the shift becomes saturated when the LUMO edge is aligned with the Fermi level. After the saturation, the LUMO intensity decreases monotonically, while a gap state grows in the valence spectra. The evolution of the LUMO gives direct evidence for the origin of the doping-induced gap state in CuPc molecules. The intensity of the LUMO, as well as the gap state, for high Cs doping ratios clearly suggests that multiply charged CuPc species are formed in the doped film.
selectivity/sensitivity can be enhanced by incorporating organic receptors. Significant dipole moments such as ketones and alcohols. We will describe the physics of operation of such sensors in various modes and also outline how the integration of organic and inorganic oxides such as SnO₂/xerogel can be achieved using a variety of techniques. The films were grown in-situ, using organic molecular beam deposition. The C and N K-edge spectra display similarities with those from other metal-Pcs, while the O K-edge and Ti L-edge spectra support the premise that the titanyl species are spatially isolated. Good agreement is found between a calculation of the partial density of states and the measured spectra. The Ti L-edge spectra display marked differences with previous reports. Two energy-loss features are reported from resonant x-ray inelastic scattering of the Ti L-edge associated with Ti 3d-O 2p and Ti 3d-N 2p charge transfer transitions. Our measurements will be discussed in the context of earlier soft x-ray studies of TiO₂, with particular attention paid to issues of contamination and beam damage.

1 Experiments performed at the NSLS, and supported in part by the AFOSR and DOE.

9:12AM P22.00005 Charge transport mechanisms in phthalocyanine thin films. CORNELIU COLENSIUC, AMOS SHARONI, IVAN K. SCHULLER, Department of Physics, University of California San Diego, La Jolla, CA 92033 — Devices consisting of phthalocyanine thin films sandwiched between gold electrodes were fabricated by organic molecular beam deposition. Samples with different organic layer thicknesses were deposited on sapphire substrates in-situ, using a shadow mask and a mobile sample holder controlled manually. The structural asymmetry of the devices determined by the different metal-organic interfaces is reflected in the I-V curves at positive and negative voltages. The logarithmic scale I-V plots can be fitted with linear functions of different slopes corresponding to different conduction regimes. At low temperatures a transition from the ohmic regime to a slope two space charge limited conduction mechanism is followed at higher voltages by a high slope linear dependence that tends to saturate when the voltage reaches maximum values. At higher temperatures the intermediary space charge limited regime disappears and the transition is from ohmic to high slope space charge limited. Traps with different energy and energy distribution determine the different conduction regimes. Shallow traps located at discrete energy levels control the transport at intermediate voltages while exponentially distributed traps determine the high voltage behavior. Work supported by AFOSR-MURI.

9:24AM P22.00006 Soft X-Ray Spectroscopic Studies of the Electronic Structure of Aluminum tris-8-hydroxyquinoline (Alq₃). A. DEMASI, L.F.J. PIPER, Y. ZHANG, I. REID, S. WANG, K.E. SMITH, Boston University, J. DONNES, Macquarie University, N. PELTEKIS, C. MCGUINNESS, Trinity College Dublin, A. MATSUURA, In-Q-Tel — The valence and core level electronic structure of the organic semiconductor aluminum tris-8-hydroxyquinoline (Alq₃) has been measured using synchrotron radiation-excited resonant x-ray emission spectroscopy (RXES), and x-ray photoelectron spectroscopy (XPS). Samples were in the form of thin films, grown in-situ in an organic molecular beam deposition chamber attached to the spectrometer system. The films were found to be highly sensitive to photon induced beam damage, but this problem could be alleviated by continuous translation of the films during measurement. Our RXES measurements are compared to the results of density functional theory (DFT) calculations. The DFT calculated C, N and O partial densities of states are found to agree very well with the corresponding emission spectra. Our measurements will be discussed in the context of earlier soft x-ray studies of Alq₃, with particular attention paid to issues of beam damage.

1 Experiments performed at the NSLS, and supported in part by the U.S. Air Force Office of Scientific Research.

9:36AM P22.00007 High Carrier Density and High Hole Mobilities of Ion Gel Gated Polymer Thin-Film Transistors. JIYOUN LEE, C. DANIEL FRIEBIE,1 Department of Chemical Engineering and Materials Science, University of Minnesota, TIMOTHY P. LODGE, Departments of Chemistry and Chemical Engineering and Materials Science, University of Minnesota — We report the comprehensive study of a highly conductive polymer thin-film transistors (IG-PTFT), in which POT-12 was used as the active ion gel comprising a polymeric network swollen with an ionic liquid as the gate dielectric. The high capacitance of ion gels (>10 μF/cm²) can induce a very large hole density (~2 x 10¹⁴ charges/cm²) in the channel of polymer semiconductor layers in IG-PTFTs, leading to low operation voltages, high hole mobilities of > 1 cm²/Vs, and high ON currents. High ionic conductivities of ion gels (> 1 mS/cm) enable fast response time (~1.5 ms at 80 % ON/OFF) of IG-PTFTs. Temperature dependent measurements were carried out with IG-PTFTs. In the high temperature range (310 K ~ 360 K), the device showed faster response time and little hysteresis due to increasing ionic conductivity with the operating temperature. At low temperature (20 K ~ 185 K) where the ions are immobile, high ON currents between source and drain can be maintained with weak temperature dependence. Overall, the results demonstrate that the IG-PTFTs offer opportunities to probe transport of high 2-D charge carrier densities in semiconductors.

1 Corresponding Author.

9:48AM P22.00008 Ionic-doping-induced nonvolatile switching in conductive polymer/inorganic complex for nonvolatile memory. QIANXI LAI, YONG CHEN, Department of Mechanical & Aerospace Engineering, University of California-Los Angeles — Organic nonvolatile memories have received extensive attention in recent years due to their low cost and high scalability. We have studied the nonvolatile switching property of a metal/conductive polymer (MEHPPV)/metal system which is induced by ionic doping under electric field. The switching phenomenon have been observed both in devices doped by electrochemical doping in liquid solution (TBAl) and in devices integrated with a solid electrolyte (RbAg4I5) in the device structure. The device can be switched from its high-resistance state (OFF) to its low resistance state (ON) by a threshold voltage with appropriate polarity and vice versa. The switching on/off ratio is more than 3 orders of magnitude with a switching time as short as 1us and the switching is reversible and repeatable. The resistance change is attributed to the reversible p-type doping of MEH-PPV by injecting/extracting iodide anions into/from the conductive polymer under the voltage bias above certain threshold amplitude. The results of Capacitance-Voltage (CV) measurements also indicated the ion migration in the polymer under the electric field.

10:00AM P22.00009 Chemical Vapor Sensing Using Dual Channel Hybrid Organic/Inorganic Field-Effect Transistors. SHANNON LEWIS, The University of Texas at Austin, SEBASTIAN SCHOEFER, The University of Texas at Austin, DEEPAK SHARMA, ANANTH DODABALAPUR, The University of Texas at Austin — We have developed a field-effect chemical sensing device architecture in which two semiconducting channels are employed, one of which is exposed to the analyte and is chemically sensitive. The second channel (usually silicon) is used for signal transduction/amplification. Such sensors work can work in many device modes including one that can be described as a “chemical memory mode”. For the chemically sensitive channel, several classes of materials can be employed including small molecule organic semiconductors, conjugated polymers, and inorganic oxides such as SnO₂. With organic semiconductor channels, it is possible to demonstrate charge trapping of volatile organic molecules with significant dipole moments such as ketones and alcohols. We will describe the physics of operation of such sensors in various modes and also outline how the selectivity/sensitivity can be enhanced by incorporating organic receptors.
10:12AM P22.00010 Correlation of microstructure and magnetotransport in organic semiconductor spin valve structures†. Y. LIU, J. GORHAM, T. LEE, H. FAIRBROTHER, H. E. KATZ, D. H. REICH, The Johns Hopkins University, S. WASTON, J. BORCHERS, NIST — Magnetic/electric devices based on organic semiconductors (OSC) hold promise due to the long spin relaxation time and the ability to tune relevant properties such as interface barriers. However, it is unclear to date whether magnetotransport effects observed in these systems is due to tunneling, or whether spin-coherent diffusive transport is also possible. We have studied magnetotransport in Co/OsC/Fe trilayer junctions, with 50 to 150 nm thick OSC layer, where tunneling would not be expected. Positive magnetoresistance (MR) is observed at T = 4.2 K for several OSCs and it persists up to T = 290 K for two systems: tris(8-hydroxyquinoline) Aluminum (III) (Alq3) and copper phthalocyanine (CuPc). In order to probe the origins of MR, we have done structural studies on Co/Alq3/Fe trilayer films by x-ray reflectivity and Auger depth profiling. The results indicate well-defined layers with modest interface roughness (3-5 nm) between the Alq3 and the surrounding FM layers. While these results rule out large-scale intermixing of Co or Fe into the OSC, they do not as yet rule out the existence of local defects, such as pinholes, in the OSC layers that could enable tunneling to occur.

†Work Supported by NSF Grant No. DMR-0520491.

10:24AM P22.00011 EPR Studies of Highly Interconnected Nanostructured Polyaniline Network†. OLUDUROTIMI O. ADETUNJI, N.-R. CHIOU, N.P. RAJU, A.J. EPSTEIN, Department of Physics, The Ohio State University, Columbus, OH 43210-1117 — We present temperature-dependent X-band electron paramagnetic resonance susceptibility and linewidth studies of nanostructured polyaniline doped with perchloric acid (PANN/HClO4). From analysis of the EPR data we determine that network has both Pauli- and Curie-like susceptibility with X’ of ~2 x 10^-5 emu/mole-2-ring repeat unit and a localized spin density of ~1 spin per 400 2-ring repeat units and exhibits a Lorentzian-like lineshape. The EPR linewidth from 100 K to room temperature exhibits two different linear regimes, where the linewidth increases linearly with increase in temperature. We will discuss the role of Korrina relaxation in determining the high temperature linewidth. We will consider the roles of disorder, localization and interfiber contact within the nanostructure network.

†This work is supported in part by the NSF-IGERT Grant No. 0221678 and NSF-NSEC Grant No. 6000644.

10:36AM P22.00012 Capacitance-voltage characterization of polythiophene-based field-effect transistors. BEHRANG HAMADANI, NIST, IAIN MCCULLOCH, Imperial College, MARTIN HEENEY, Queen Mary University of London, DAVID GUNDLACH, NIST, NIST COLLABORATION, IMPERIAL COLLEGE COLLABORATION — We report on frequency-dependent capacitance-voltage characteristics of organic field-effect transistors based on (2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-b]thiophene) as the active polymer layer. The gate voltage and frequency behavior of the devices with the polymer spun on treated and untreated oxide gate dielectric are explored. The high quality of the devices (contact and channel properties) allows the use of traditional CV modeling to accurately describe the electronic characteristics of the intrinsic channel. The findings from this study provide new insight into charge trapping and transport in the field-accumulated channel of organic field-effect devices.

Wednesday, March 12, 2008 8:00AM - 10:24AM –
Session P23 DMP GMAG: Focus Session: Multifunctional Oxides: BiFeO3 and Thin Films

8:00AM P23.00001 Strain tunability and domain structures of epitaxial (001) BiFeO3 thin films†. CHANG-BEOM EOM, University of Wisconsin-Madison — It was recently discovered that the spontaneous polarization (P_s) values determined in epitaxial BiFeO3 thin films, ~100 μC/cm^2, are over an order of magnitude higher than those previously measured in bulk samples. This raises a fundamental question: can the remanent polarization and other properties of BiFeO3 be tuned by strain? We studied the strain dependence of remanent polarization and domain structures of BiFeO3 through direct measurements on the same epitaxial (001)_p BiFeO3 thin-film capacitors before and after releasing them from an underlying Si substrate. Our measurements reveal that: (1) the large P_s of BiFeO3 is indeed intrinsic; (2) the out-of-plane polarization (P_P) of (001)_p-oriented BiFeO3 thin films has a strong strain dependence. These findings can be exploited in studying symmetry-dependent magnetoelectric coupling of BiFeO3, where strain and/or symmetry play a role in the coupling because the direction of magnetic spin ordering is not parallel to that of ferroelectric polarization switching.


8:36AM P23.00002 Local Electrical Conductivity of Multiferroic Domain Walls. QING HE, JAN SEIDEL, LANE MARTIN, YING-HAO CHU, QIAN ZHAN, FENG WANG, RAMAMOORTHY RAMESH, UC Berkeley — There is an intense interest in magnetoelectric coupling between electric and magnetic due to its potential to the revolutionary device architectures. Single-phase multiferroics - materials that show spontaneous magnetization and polarization simultaneously at ambient conditions - remain elusive as most systems (such as the manganites) exhibit magnetoelectric coupling between electric and magnetic due to its potential to the revolutionary device architectures. One multiferroic material, however, has played a key role in rejuvenating the field after a report of multiferroicity only at low temperatures. Alternatively, multiferroics can be synthesized as a composite system, e.g. as a product property of a composite phase consisting of a magnetostriective and a piezoelectric material. One multiferroic material, however, has played a key role in rejuvenating the field after a report of large ferroelectric polarization combined with interesting magnetic properties - BiFeO3, consisting of a magnetostrictive and a piezoelectric material. One multiferroic material, however, has played a key role in rejuvenating the field after a report of multiferroicity only at low temperatures. Alternatively, multiferroics can be synthesized as a composite system, e.g. as a product property of a composite phase consisting of a magnetostriective and a piezoelectric material. One multiferroic material, however, has played a key role in rejuvenating the field after a report of large ferroelectric polarization combined with interesting magnetic properties - BiFeO3. Here we provide evidence of a unique property of single domain walls in multiferroic BiFeO3. Unlike other multiferroic materials, e.g. PbTiO3, on which the electronic properties of the domain walls are not significantly different from the domain area, we observe a finite electric conductivity at room temperature in ferromagnetic domain walls using conductive atomic force microscopy. This intrinsic property of the domain wall is attributed to a changed crystallographic structure as revealed by high resolution transmission electron microscopy. Additionally, optical absorption measurements confirm a change in bandstructure at domain walls in BiFeO3.

8:48AM P23.00003 The multiferroic properties of Bi(Fe1/2Cr1/2)O3 compound. CHANGQING JIN, J.L. ZHU, H.X. YANG, S.M. FENG, L.J. WANG, R.C. YU, X.H. WANG, L.T. LI. Institute of Physics, Chinese Academy of Sciences, Beijing, China — Dense Bi(Fe1/2Cr1/2)O3 ceramics of R3c crystal structure were synthesized by solid state reaction under high pressure. TEM observations reveal superstructure characteristics in Bi(Fe1/2Cr1/2)O3. Magnetization as well as dielectric properties of Bi(Fe1/2Cr1/2)O3 ceramics were characterized over a broad temperature.
9:00AM P23.00004 Optical coupling to spin waves in the cycloidal multiferroic BiFeO₃. ROGERIO DE SOUSA, Department of Physics, University of California, Berkeley, CA, USA, JOEL E. MOORE, Department of Physics, University of California, and Department of Materials Science, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — The magnon and optical phonon spectrum of an incommensurate multiferroic such as BiFeO₃ is considered in the framework of a phenomenological Landau theory. The resulting spin wave spectrum is quite distinct from commensurate substances due to soft mode anisotropy and magnon zone folding. The former allows electrical control of spin wave propagation via reorientation of the spontaneous ferroelectric moment. The latter gives rise to multiple magneto-dielectric resonances due to the coupling of optical phonons at zero wavevector to magnons at integer multiples of the cyclod wavevector. These results show that the optical response of a multiferroic reveals much more about its magnetic excitations than previously anticipated on the basis of simpler models.

3This work was supported by the Western Institute of Nanoelectronics (RdS) and by NSF DMR-0238760 (JEM).

4Current Address: Dept. of Physics and Astronomy, University of Victoria, B.C., Canada

9:12AM P23.00005 Electric Field Controlled Magnetism in BiFeO₃/Ferromagnet Films. M.B. HOLCOMB, Y.H. CHU, L.W. MARTIN, M. GAJEK, J. SEIDEL, R. RAMESH, UC Berkeley, A. SCHOLL, Advanced Light Source, LBNL, A. FRAILE-RODRIGUEZ, Swiss Light Source, PSI — Electric field control of magnetism is a hot technological topic at the moment due to its potential to revolutionize today’s devices. Magnetoelectric materials, those having both electric and magnetic order and the potential for coupling between the two, are a promising avenue to approach electric control. BiFeO₃, both a ferroelectric and an antiferromagnet, is the only single phase room temperature magneto-electric that is currently known. In addition to other possibilities, its multiferroic nature has potential in the very active field of exchange bias, where an antiferromagnetic thin film pins the magnetic direction of an adjoining ferromagnetic layer. Since this antiferromagnet is electrically tunable, this coupling could allow electric-field control of the ferromagnetic magnetization. Direction determination of antiferromagnetic domains in BFO has recently been shown using linear and circular dichroism studies. Recently, this technique has been extended to look at the magnetic domains of a ferromagnetic grown on top of BFO. The clear magnetic changes induced by application of electric fields reveal the possibility of electric control.

9:24AM P23.00006 Investigation of domain walls in multiferroic BiFeO₃. JAN SEIDEL, LANE MARTIN, YING-HAO CHU, QIAN ZHAN, QING HE, Department of Materials Science and Engineering and Department of Physics, UC Berkeley, FENG WANG, Department of Physics, UC Berkeley, RAMAMOORTHY RAMESH, Department of Materials Science and Engineering and Department of Physics, UC Berkeley, AXEL ROTHER, NICOLA SPALDIN, Materials Department, UC Santa Barbara, GUSTAV CATALAN, JAMES SCOTT, Department of Earth Science, University of Cambridge, UK — We present a thorough study of domain walls in multiferroic BiFeO₃ thin films using scanning probe methods, transmission electron microscopy, transport measurements coupled with theoretical studies. In rhombohedral BiFeO₃, three different domain wall orientations exist, namely 180, 109, and 71 degrees. We find that the domain configurations in thin films are strongly dependent on the processing conditions. Here we investigate electrical and structural properties of all three varieties. Atomic resolution STEM studies were used to reveal the structure across the domain walls, with a specific focus on 109°. We observe that the changed crystallographic structure in domain walls gives rise to a change in local properties. From the investigation of individual domain walls we also infer their relation to changed macroscopic properties in thin films. This work is supported by the US DOE, ONR MURI, NSF Chemical Bonding Center program, and the Alexander von Humboldt Foundation.

9:36AM P23.00007 Optical properties of BiFeO₃ thin films and single crystal. R.C. RAI, X.S. XU, T.V. BRINZARI, J.L. MUSFELDT, University of Tennessee, D.J. SINGH, Oak Ridge National Laboratory, S. LEE, S-W. CHEONG, Rutgers University, Y.H. CHU, R. RAMESH, University of California, Berkeley, S. MCGILL, National High Magnetic Field Laboratory — BiFeO₃ has been studied using optical and magneto-optical spectroscopy and the results are compared with first-principle calculations. The optical gap in thin films (2.7 eV) is much larger than that in the single crystal (1.3 eV), the evidence that this system has a novel transition between strongly correlated and band insulator behavior. Both magnetic field and temperature suppress the excitation between the strongly hybridized valence levels and Fe d levels near 1.5 eV. The temperature and magnetic field effects appear to scale energetically suggesting spin-charge coupling. The high energy magneto-electric contrast shows a jump at 18 T corresponding to the transition from toroidal to homogeneous antiferromagnetic phase.

3This work is supported by the U.S. Department of Energy.

9:48AM P23.00008 Magnetization manipulation in multiferroic devices. MARTIN GAJEK, LANE MARTIN, YING HAO CHU, MARK HUIJBEN, MICKY BARRY, RAMAMOORTHY RAMESH, UNIVERSITY OF CALIFORNIA, BERKELEY TEAM — Controlling magnetization by purely electrical means is a central topic in spintronics. A very recent route towards this goal is to exploit the coupling between multiple ferroic orders which coexist in multiferroic materials. BiFeO₃ (BFO) displays antiferromagnetic and ferroelectric orderings at room temperature and can thus be used as an electrically controllable pinning layer for a ferromagnetic electrode. Furthermore, BFO remains ferroelectric down to 2nm and can therefore be integrated as a tunnel barrier in MTJ’s. We will describe these two architecture schemes and report on our progresses towards the control of magnetization via the multiferroic layer in those structures.

10:00AM P23.00009 Electronic and magnetic structures of double perovskite multifunctional La₃NiMnO₁₀ thin films. HAIZHONG GUO, JIANDI ZHANG, Department of Physics, Florida International University, Miami, FL 33199, ARUNAVA DE SOUSA, Center for Materials for Information Technology and Department of Chemistry, University of Alabama, Tuscaloosa, Alabama 35487, M. VARELA, S.J. PENNYCOOK, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 — Electronic and magnetic structures of the ordered double perovskite La₃NiMnO₁₀ (LNMO) thin films grown by pulsed laser deposition have been studied by x-ray absorption spectroscopy (XAS) and magnetic circular dichroism spectroscopy (XMCD). Based upon the results of XMCD, we find that the primary ion valence states to be Mn⁴⁺/Ni⁴⁺, and the ferromagnetism resulting from Mn⁴⁺ O 2⁻ Ni⁴⁺ superexchange interaction. Additionally, we show that the LNMO samples contain some Mn⁴⁺ and Ni³⁺ Jahn-Teller ions caused by oxygen or cation related defects. The orbital and spin magnetic moments of the Mn 3d and Ni 3d also have been deduced from the magneto-optical sum rules and compared with magnetization measurements.

1Supported by NSF DMR-0346826, NSF NIRT Grant No. CMS-0609377, and DOE DE-FG02-04ER46125.
10:12AM P24.00010 Influence of oxygen concentration on the magnetic properties of multi-functional La$_2$CoMnO$_6$, thin films. ARUNAVA GUPTA, Center for Materials for Information Technology and Department of Chemistry, University of Alabama, Tuscaloosa, Alabama 35487, HAIZHONG GUO, JIAN DI, JIANGI ZHANG, Department of Physics, Florida International University, Miami, FL 33199, M. VARELA, S.J. PENNYCOOK, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 — The dependence of the magnetic properties on oxygen concentration in epitaxial La$_2$CoMnO$_6$(LCMO) thin films has been investigated grown by pulsed laser deposition (PLD). Using x-ray magnetic circular dichroism spectral microscopy (XMCD) at Mn$_{L2,3}$ and Co$_{L2,3}$ edges, we have determined that the primary ion valence state is Mn$^{3+}$/Co$^{3+}$. Additionally, we see evidence of some low-spin Co$^{4+}$ ions, corresponding to the existence of a second ferromagnetic (FM) phases in our samples. The existence of oxygen vacancies induces the local vibronic Mn$^{3+}$/Co$^{3+}$ superexchange interactions in direct competition with the static FM Mn$^{3+}$/Co$^{3+}$ interactions. This results in the appearance of a new low temperature FM phase and suppression of the high-temperature FM phase, creating two distinct magnetic phase transitions.

1Supported in part by NSF DMR-0346826, NSF NIRT Grant No. CMS-0609377, and DOE DE-FG02-04ER46125.

Wednesday, March 12, 2008 8:00AM - 10:36AM – Session P24 DMP: Focus Session: Optical Properties of Nanostructures V: Plasmonics and Metallic Nanostructures Morial Convention Center 216

8:00AM P24.00001 Calculations of second harmonic generation by nano-particles or holes. WILLIAM SCHAICH, Indiana University — We are setting up finite-difference time-domain (fDTD) calculations of second harmonic generation (SHG) by metallic nano-particles or at nano-holes in metallic films. This generation is driven by first order fields at the metal surfaces, using the phenomenological a and b parameters that have been used to describe shg at planar jellium-metal surfaces. Our interest is in locating and understanding the occurrence of resonances and hot-spots for shg.

1Research supported in part by NSF-CBET-0708590.

8:12AM P24.00002 Plasmonic bonding and anti-bonding forces in a bisphere. TSZ FAI (JACK) NG, C.T. CHAN, The Hong Kong University of Science and Technology — By exciting the surface plasmon resonance of a pair of nanoparticles using intense laser illumination, one can exploit huge optical forces on the nanoparticles. We calculate such resonant optical force using a multiple scattering and Maxwell stress tensor formalism, which is "exact" within the classical electrodynamics. It is shown that the full electrodynamic calculation can give results that differ significantly from those obtained by the quasi-static approximation. As the pair of nanoparticles approach each other, the individual particle's plasmonic modes hybridize and split into bonding and anti-bonding modes, which induced attraction and repulsion respectively. At very small separations, the bonding (anti-bonding) modes are forced to curve downward (upward) in frequency significantly, resulting in the formation of a low frequency attractive (high frequency repulsive) band. Consequently, a low frequency laser illumination will induce strong attraction, promoting particle clustering, and a high frequency illumination will induce strong repulsion, preventing particle aggregation. With high intensity, these resonant forces can dominate over the other relevant forces, including the van der Waals force, when the separation between the particles is several nanometers.

8:24AM P24.00003 Surface-enhanced Raman Scattering from Virus-like Particle Crystals. CHRISTOPHER DUFORT, BOGDAN DRAGNEA, Indiana University, Department of Chemistry — Recently, a method for the encapsidation of gold nanoparticles by an icosahedral virus protein coat, termed a virus-like particle (VLP), has been developed. Of particular interest is in observing their spectroscopic properties upon arrangement into a three-dimensional crystal lattice. Here we present the surface-enhanced Raman scattering spectrum of such an assembly. This is made possible by the plasmonic coupling of adjacent gold nanoparticles when excited near their plasmon resonant frequency. To determine whether the SERS effect is arising from isolated hot spots or a large number of junctions acting in unison we employed scanning confocal Raman spectroscopy. This seems to indicate the latter, as a uniform Raman intensity is observed across entire crystals.

8:36AM P24.00004 The effects of nanoparticle spacing on second-harmonic generation from gold nano-dimers. DAVON W. FERRARA, KEVIN A. TETZ, MATTHEW D. MCMAHON, RICHARD F. HAGLUND, JR., Vanderbilt University — Second-generation harmonic (SHG) is an important signature of electron dynamics in nanoparticles (NPs) as well as a sensitive probe of surface effects. In the gap between closely spaced pairs of NPs, or nanodimers (Nds), localized electromagnetic field energy creates a hot spot that has been shown to affect SHG from asymmetric Nds. We will present new experimental results demonstrating the role that gap size and field localization plays in SHG from centrosymmetric arrays of gold Nds. Using standard electron-beam lithography techniques, NPs were made 20 nm in height with varying areal aspect ratios. In the ND arrays, symmetry forbids SHG in the forward direction, but not at larger angles. Our experiments indicate suppression of SHG intensity with decreasing gap size and evidence of stronger long-range interactions between NPs with separation over 200 nm. Finite-difference time-domain simulations were also performed in order to correlate field localization with SHG. Our simulations show a strong dependence on the polarization of incident light.

1Supported in part by DOE grant DE-FG02-01ER45916.

8:48AM P24.00005 Optical Imaging Properties of Metal Nanoparticle Chains. DAVID CITRIN, Georgia Institute of Technology — Chains of noncontacting noble-metal nanoparticles are known to support coupled plasmonic-electromagnetic modes known as plasmon polaritons, in which those polarized perpendicular to the chain axis exhibit group and phase velocity in opposite directions. This in turn has attracted interest in nanoparticle chains and arrays as left-handed materials for optical applications. In this contribution, I discuss recent work in my group on the imaging properties of nanoparticle chains. In particular, I present work that demonstrates theoretically the focusing properties of nanoparticle chains. I further discuss possible applications in near-field optics.

9:00AM P24.00006 Plasmonic superfocusing on metallic tips for near-field optical imaging and spectroscopy. CATALIN C. NEACSU, ROB OLMON, SAMUEL BERWEGER, ALEXANDRIA KAPPUS, FRIEDRICH KIRCHNER, Department of Chemistry, University of Washington, Seattle, USA, CLAUS ROPERS, Max-Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, Germany, LAX SARAF, Pacific Northwest National Laboratory, Richland, WA, USA, MARKUS B. RASCHKE, Department of Chemistry, University of Washington, Seattle, USA — Realization of localized light sources through nonlocal excitation is important in the context of plasmon photonics, molecular sensing, and in particular near-field optical techniques. Here, the efficient conversion of propagating surface plasmons, launched on the shaft of a scanning probe tip, into localized plasmon at the apex provides a true nanoconfined light source. Focused ion beam milling is used to generate periodic surface nanostructures on the tip shaft that allow for tailoring the plasmon excitation. Using ultrashort visible and mid-IR transients the dynamics of the propagation and subsequent scattered emission is characterized. The strong field enhancement and spatial field confinement at the apex is demonstrated studying the coupling of the tip in near-field interaction with a flat sample surface. It is used in scattering near-field spectroscopic imaging (s-SNOM) to probe surface nanostructures with spatial resolution down to 10 nm.
Novel properties of nanostructured metal particles and films. SHENGLI ZOU, University of Central Florida — Using electromagnetic dynamics, we simulate the extinction spectra and enhanced electric fields of nanostructured metal nanoparticles and films. Their sensing and waveguide applications will be discussed. The sensing of molecules is achieved by the shift of the plasmon resonance wavelength of nanoparticles or enhanced Raman scattering or fluorescence signals, which are due to the enhanced local electric fields near or far away from the metal surface. The waveguide is achieved by the electromagnetic coupling in a one dimensional particle chain or a perforated metal film.

Resonance of metallic wire structures. LEI ZHOU, Y. ZHANG, Fudan University, SIU TAT CHUI, University of Delaware — Metallic wire structures form a common class of physical systems. We illustrate how to understand the general physics of the wire systems with a specific example, the split ring resonator. We derived simple polynomial equations to determine the entire resonance spectra of split ring structures, which can be analytically solved in the limit of narrow wires. A resonance spectrum very similar to that of a straight wire is obtained. For double stacking split rings made with flat wires, we showed that the resonance frequency depends linearly on the ring-ring separation. In particular, we found that the wavelength of lowest resonance mode can be made as large as 10^3, the geometrical size of the ring for realistic experimental conditions, whereas for current systems this ratio is of the order of 10. Finite-difference-time-domain simulations on realistic structures verify the analytic predictions.

Fabrication of Plasmonic Optical Probe and Its Characterization. SEONG SOO CHO, SunMoon University, D.W. KIM, VINAYAH JHA, O. SUWAL, SunMoon Univ, M.J. PARK, Korea Military Academy, RESEARCH CENTER FOR NANOSCIENCE, NATIONAL RESEARCH LAB TEAM — Recently, there have been tremendous interests about the nano-structured optical probe using surface plasmon polariton due to possible applications of the next generation local communication devices and nano-bio sensor technology. The nano-size metallic apertures such as metal-coated fiber probe and microfabricated pyramidal probe, have shortcomings of very low output intensities. With periodic groove or defects near the aperture on the microfabricated pyramidal probe, the huge output intensity enhancement has been reported [1]. In this talk, the fabrication with nano-flowers including metallic scattering centers around the nano-size aperture and its optical characterization of the pyramidal metallic probe will be presented. References: [1] The effect of groove shape on light transmission, S.S. Choi, etc., 3rd International Conference on Surface Plasmon Photonics, June 17-22, Dipon, France.

Inter-particle coupling and polarizability of silver nanoparticle dimers. KE ZHAO, CLAUDIA TROPAREVSKY, University of Tennessee & Oak Ridge National Laboratory, ADOLFO EGUILUZ, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee, THEORETICAL CONDENSED MATTER PHYSICS AT UNIVERSITY OF TENNESSEE & OAK RIDGE NATIONAL LABORATORY COLLABORATION — Using a real-space implementation of density-functional theory, we investigate systematically the electronic/chemical coupling of two silver nanoparticles of varying sizes. The nanoparticles are allowed to approach each other along two distinct directions defined by, respectively, maximum and minimum static polarizabilities. We show that, as the inter-particle separation decreases, the static polarizability of the dimer shows signatures of crossover to a strong-coupling regime. Moreover, we analyze the connection between the crossover from weak to strong coupling regimes of the nanoparticles and the electron density overlap from the states contributed by the individual nanoparticles. The significance of these results will be discussed in connection with the prevailing theories of the electromagnetic enhancement of surface-enhanced Raman scattering.

Enhancement of Light Transmission through Bull’s Eye Structures. SINAN SELCUK, Department of Physics University of Florida, DANIEL ARENAS, DAVID B. TANNER, ARTHUR F. HEBARD, Department of Physics University of Florida — Optical transmission of a single hole in a metal film surrounded by concentric surface grooves is shown to have an enhanced transmission. We fabricated these structures in silver films which are thin enough to let light through without a center hole. We have measured the optical transmission and reflection in visible to near infrared spectrum observing enhanced transmission scaling with groove periodicity. Opening a hole in the center gives rise to destructive interference between the light passing through the structure and the light passing through the hole. We will discuss the mechanisms behind light transmission for the bullseye structure for varying hole size, groove periodicity, groove depth and the metal thickness.

Fluorescence enhancement from nominally flat surfaces. SHY-HAUH GUO, Department of Electrical and Computer Engineering, University Of Maryland, College Park, MD, 20742, HUNG-CHIH KAN, Department of Physics, University Of Maryland, College Park, MD, 20742, RAY PHANEUF, Department of Materials Science and Engineering, University Of Maryland, College Park, MD, 20742 — We report on experimental investigations of fluorescence enhancement from nominally flat silver and silicon substrates, in the presence of an oxide spacer layer. By varying the thickness of the oxide layer, we were able to change the spacing between the substrates and the oxide layer thickness. We find that the relative fluorescent intensity measured above Ag vs. Si substrates oscillates, indicating a resonant effect. We investigate the effect of nanoscale roughness on the observed fluorescent enhancement.

Anisotropic Light Scattering from Ferrofluids. CORNELIU RABLAIU, PREM VAISHNAVHA, Kettering University, Flint, MI, RATNA NAIK, GAVIN LAWES, RON TACKETT, C. SUDAKAR, Wayne State University, Detroit, MI — We have investigated the light scattering in DC magnetic fields from aqueous suspensions of Fe_3O_4 nanoparticles coated with tetra methyl ammonium hydroxide and γ-Fe_2O_3 nanoparticles embedded in alginate hydrogel. For Fe_3O_4 ferrofluid, anomalous light scattering behavior was observed when light propagated both parallel and perpendicular to the magnetic fields. This behavior is attributed to the alignment and aggregation of the nanoparticles in chain-like structures. A very different light scattering behavior was observed for γ-Fe_2O_3 alginate sample where, under the similar conditions, the application of the magnetic field produced no structured change in scattering. We attribute this difference to the absence of chain-like structures and constrained mobility of iron nanoparticles in the alginate sample. The observation is in agreement with our relaxation and dissipative heating results where both samples exhibited Neel relaxation but only the Fe_3O_4 ferrofluid showed Brownian relaxation. The results suggest that Brownian relaxation and nanoparticle mobility are important for producing non-linear light scattering in such systems. 3.P.P. Vaishnava, R. Tackett, A. Dixit, C. Sudakar, R. Naik, and G. Lawes, J. Appl. Phys. 102, 063914 (2007).

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P25 DPOLY DBP: Focus Session: DNA and Protein Analysis with Micro and Nanofluidics Morial Convention Center 217
8:00AM P25.00001 Learning from the Jersey Turnpike: Cell Lysis, Labeling and Washing with Microfluidic Metamaterials, ROBERT AUSTIN, Princeton University — Directing objects across functional streamlines at low Reynolds number is difficult but important since this motion can be used to label, lyse, and analyze complex biological objects on-chip without cross-contamination. Here we use an asymmetric post array to move cells across colloring reagents and show on-chip, immunofluorescent labeling of platelets with washing and E. Coli cell lysis with simultaneous separation of bacterial chromosome from the cell contents. Furthermore, we develop the concept of a microfluidic metamaterial by using the basic asymmetric post array as a building block for complex particle handling modes. These modular array elements could be of great use for developing robust techniques for on-chip, continuous flow manipulation and analysis of cells, large bio-particles, and functional beads.

8:36AM P25.00002 DNA Docking with Functionalized Colloidal Probes, LU ZHANG, YINGXI ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame — The docking of DNA with probe-functionalized microparticles remains inadequately understood, despite the significance of DNA hybridization-based technologies for high-throughput screening for genetic analysis and biomedical diagnostics. In this work, we employ fluorescence correlation spectroscopy (FCS) and confocal microscopy to examine DNA-colloid interaction and resulting conformational structures of DNA oligomers with oligonucleotide-functionalized colloidal probes, whose particle size varies from 100 nm to 3 um. We observe that the docking efficiency strongly depends on DNA length, colloid size and surface functionality. Optimal probe size and temperature are found for rapid hybridization. We conjecture that the resulting structure of DNA at the interface of colloidal probes is determined by both steric effects and DNA charge condensation. If time permits, we will discuss our recent work on the docking of elongated DNA with functional probes by imposed dielectrophoretic forces in the presence of AC fields.

8:48AM P25.00003 Confinement spectroscopy: A novel approach to force spectroscopy1, FREDRIK PERSSON, PAWEL UTIKO, WALTER REINSER, ANDERS KRISTENSEN, Technical University of Denmark — In physics DNA is readily described by its mechanical properties, neglecting its chemical composition. By studying variations in these properties conclusions can be drawn about the interaction between DNA and both its environment and also ligand binding to DNA. These investigations are normally performed by force spectroscopy using optical or magnetic tweezers associated with an elaborate experimental setup. We introduce confinement spectroscopy, as a complementary technique, where a continuously variable degree of spatial restriction is applied to the molecule in a fluidic funnel-like geometry. By driving the molecule along the funnel, an extension versus confinement curve is obtained. This curve contains not only information regarding the molecule elasticity, but also new details concerning the self- and surface-interactions of the molecule. It is also easily integrated into lab-on-a-chip devices.

9:00AM P25.00004 Fluorescence microscopy studies of the DNA motion near voltage biased solid-state nanopores, KAZUHIKO OBANA, YOICHI NAKAMURA, KAYA KOBAYASHI, TOSHIYUKI MITSUI, Aoyama Gakuin University — A solid state nanopore in a Si-based thin insulating membrane works as a single DNA molecule sensing device that provides the information of the length and the folding configuration of the DNA by measuring ionic currents when the DNA translocates through the pore [1]. These nanopores may play a significant role in molecular electronics and rapid DNA sequencing. Now one of the issues related to this nanopore sensing technique is clogging the nanopores by DNA molecules because it significantly extends the DNA translocation time. To elucidate this issue, we use time-resolved fluorescence microscopy to observe the DNA motion near voltage biased nanopores. We will discuss the DNA motion near nanopores under the various applied voltages. [1] J. Li M. Gershov, D. Stein, E. Brandin, and J.A. Golovchenko, Nature Materials 2: 611 (2003); T. Mitsui, D. Stein, Y.-R. Kim, D. Hoogerheide, and J.A. Golovchenko, Phys. Rev. Lett. 96: 036102-1 (2006)

9:12AM P25.00005 Influence of polymer-pore interactions on translocation, TAPIO ALA-NISSILÄ, Helsinki University of Technology, KAIYU LUO, Helsinki University of Technology, Finand, SEE-CHEN YING, Brown University, ANIKET BHATTACHARYA, University of Central Florida, TRK COLLABORATION, BROWN COLLABORATION, UCF COLLABORATION — We investigate the influence of polymer-pore interactions on the translocation dynamics using Langevin dynamics simulations2. An attractive interaction can greatly improve translocation probability. At the same time, it also increases translocation time slowly for weak attraction while exponential dependence is observed for strong attraction. For fixed driving force and chain length the histogram of translocation time has a transition from Gaussian distribution to long-tailed distribution with increasing attraction. Under a weak driving force and a strong attractive force, both the translocation time and the residence time in the pore show a non-monotonic behavior as a function of the chain length. Our simulations results are in good agreement with recent experimental data3.

9:24AM P25.00006 Nanofilters for high throughput DNA separation, NABIL LAACHI, University of Minnesota, CARMELO DECLET, University of Puerto Rico-Mayaguez, CHRISTINA MATSON, Mississippi State University, KEVIN DORFMAN, University of Minnesota — Nanofilters are a novel class of microfabricated devices for rapidly separating short, rigid DNA. The succession of alternating narrow slits (~50nm) and deep wells (~300nm) is used to trap the DNA, which then escape at a size-dependent rate. Experiments and near-equilibrium theoretical arguments both indicate that smaller DNA travel faster in a weak field, but the separation fails at around 100V/cm. We theoretically show that the speed and performance of the device can be enhanced using high fields of several hundred V/cm. Based on scaling arguments, the separation of short, rod-like DNA molecules at high fields occurs via "torque-assisted escape," which originates from the non-uniform electric field at the slit entrance. The quadratic dependence of the torque on the molecule size indicates that larger molecules will now emerge first; under a high field, the device operates in a band-inverted manner. Brownian dynamics simulation results confirm the mobility increase with size, with a quasi-plateau at very large fields.

9:36AM P25.00007 Rapid DNA Identification by Dielectrophoresis of Nanocolloids, ZACHARY GAGNON, SATYAJIYOTI SENAPATI, JASON GORDON, HSUEH-CHIA CHANG, Dept. of Chemical and Biomolecular Engineering, University of Notre Dame — Due to their size and number, dispersed oligo-functionalized nanocolloids can reduce the diffusion length/docking time and increase the sensitivity of ssDNA hybridization reactions by orders of magnitude compared to immobilized probes. We find that, for long target ssDNAs, their docked conformation is a sensitive function of the nanocolloid size, surface charge, functionalized probe density and number of docked DNAs per bead. Three distinct conformations (collapsed, stretched and condensed) are detected via independent light scattering, Zeta potential, dielectrophoresis (DEP) and electron micrograph techniques. By optimizing the hybridization conditions to produce a stretched conformation, we are able to significantly change the DEP cross-over frequency of hybridized beads, thus allowing rapid label-free detection of hybridization by simple impedance techniques down to pM concentrations.
9:48AM P25.00008 The non-driven polymer translocation through a nanopore: relaxation and translocation are not decoupled. GARY W. SLATER, MICHEL G. GAUTHIER, University of Ottawa — Most theoretical models describing the translocation of a polymer chain through a nanopore use the hypothesis that the polymer remains in an equilibrium random coil conformation during the process. In other words, models generally assume that the characteristic relaxation time of the chain is small enough compared to the translocation time that non-equilibrium polymer conformations can be ignored. We present Molecular Dynamics simulations that directly test this hypothesis by looking at the escape time of unbiased polymer chains starting with different initial conditions. We find that the chains are deformed for the systems studied, even though the translocation time is about 10 times larger than the relaxation time. Our most striking result is the observation that the last half of the chain escapes in less than 12% of the total escape time, which implies that there is a large entropy-driven acceleration of the chain at the end of its escape from the channel.

10:00AM P25.00009 Digital DNA: Physics of DNA in Nanoparticle Lattices. WALTER REISNER, Brown University Dept. of Physics, JONAS TEGENFELDT, Dept Physics / Solid State Physics Lund University, NIELS LARSEN, Biosystems/Polymer Dept. Risø National Laboratory Technical University of Denmark, HENRIK FLYVBJERG, Biosystems Dept. Risø National Laboratory Technical University of Denmark, DEREK STEIN, Dept. of Physics Brown University, ANDERS KRISTENSEN, MIC - Department of Micro and Nanotechnology Technical University of Denmark — Controlling the on-chip organization and conformation of DNA is important for a number of interrelated nanotechnology disciplines. We introduce a new type of nanostructure consisting of a nanoplat with a built in spatial modulation of confinement created by arrays of embedded nanoparticles. Nanoplates are square plates with 100 nm wide and 500 nm deep. We show that DNA molecules inserted into such nanostructures can adopt conformational states that can be used to store and retrieve information. A further application of this type of structures is that they will spontaneously adopt a 'digitized' conformation consisting of filled nanoplates connected by fluctuating links. By adjusting the spacing, organization and placement of the nanoparticles it is possible to immobilize DNA at predetermined regions of device without additional chemical modification and achieve a high degree of control over local DNA conformation. We will present results from fluorescence microscopy experiments on the equilibrium behavior and dynamics of DNA in such structures and interpret these results in terms of a simple statistical mechanical model.

10:12AM P25.00010 Dynamics of DNA molecules confined to slit-like nanofluidic channels. CHRISTINE MEYER, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, DOUWE JAN BONTHUIS, present address: Technical University of Munich, Germany, DEREK STEIN, present address: Brown University, USA, CEES DEKKER, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — We experimentally investigate the dynamics of DNA in confined spaces. This is not only important for a better understanding of the behavior of DNA as a biologically relevant molecule but also helps us to test general polymer dynamics models. Fluorescently stained DNA molecules are inserted into slit-like nanofluidic channels. The channel material is fused silica and the channels are fabricated using a bonding process. We take fluorescent images of the DNA in channels of different heights and measure the projected size of the DNA molecules fitted by an ellipse. Furthermore, we measure the relaxation times derived from the autocorrelation function of the size. If the channel height is smaller than twice the radius of gyration of the DNA molecules ($R_g = 700$ nm) both parameters agree with the predictions of de Gennes. For even smaller channels with a height less than twice the persistence length of stained DNA ($L_p = 60$ nm) the dynamics resemble the predictions made by Odijk for this regime.

10:24AM P25.00011 Electrokinetic transport at a nanocapillary/microchannel interface. JARROD SCHIFFBAUER, KATHLEEN KELLEY, BOYD EDWARDS, AARON TIMPERMAN, West Virginia University — Coupled electrokinetic transport phenomena play a central role in concentration polarization near the interface between a permselective nanocapillary membrane and a microchannel. Here the effects of ion concentration and potential distribution on transport through a single nanocapillary are studied using both semi-empirical and fundamental models. The fundamental models are developed within the context of the coupled electrohydrodynamic transport equations for multiple charged species in aqueous solution. The semi-empirical models describe average species and fluid fluxes through the respective regions.


10:48AM P25.00013 Separation of DNA in nanoscale devices with alternating channel depth. HENRY LAU, ELIZABETH STRYCHALSKI, HAROLD CRAIGHEAD, LYNDEN ARCHER, Cornell University — The size-dependent separation of DNA using nanofabricated devices consisting of alternating deep and shallow regions have been the subject of numerous experimental and theoretical works. Recent Brownian dynamics simulations suggest that the separation of rigid-rod DNA can be effected at high electric fields without a loss of resolution (PRL, 2007, 98, 098106). To study the dynamics of DNA separation at high fields, electrophoresis experiments were carried out using DNA fragments up to 753 bp in size. As the transport mechanism of DNA fragments in gels has been shown to be a strong function of topology (Electrophoresis, 2004, 25, 1772), electrophoresis of branched rigid-rod DNA molecules was performed to investigate the effects of aneute architecture on mobility in nanofabricated devices. By comparing the mobility of branched and linear DNA molecules of identical total molecular weight, we exclude the influence of size and charge and focus on the effects of branch size and location, and overall aneute topology. Our results help elucidate the electrophoretic migration mechanism of DNA molecules with complex architecture in sieving media with precisely-controlled internal structures.

Wednesday, March 12, 2008 8:00AM - 10:48AM — Session P26 DCP: Focus Session: Quantum Control III — Morial Convention Center 218

8:00AM P26.00001 Use of Ultrafast Molecular Dynamics and Optimal Control for Identifying Biomolecules. JEAN-PIERRE WOLF, University of Geneva — With F. COURVOISIER, L. GUUYON, V. BOUTOU, and M. ROTH, H. ROSLUND, H. RABITZ, Princeton University. The identification and discrimination of molecules that exhibit almost identical structures and spectra using fluorescence spectroscopy is considered quite difficult. In order to evaluate the capability of optimal control for discriminating between the optical emissions of nearly identical molecules, we developed a new approach called ‘optimal dynamic discrimination’ (ODD). A proof of principle ODD experiment has been performed using Riboflavin (RBF) and Flavin Mononucleotide (FMN) as model system. We used a complex multipulse control field made of a pair of pulses (UV and IR). The UV part ($\lambda = 400$ nm) is optimally shaped using a control learning loop while the IR component (800 nm) is FT-limited (100 fs) and set at a definite time delay with respect to the UV pulse. Clear discrimination was observed for optimally shaped pulses, although the linear spectra from both molecules are virtually identical. A further experiment showed that, by using the optimal pulse shapes that maximize the fluorescence depletion in FMN and RBF in a differential manner, the concentration of both molecules could be retrieved while they were mixed in the same solution. The ODD demonstration sets out a promising path for future applications, as for example fluorescence microscopy where endogenous fluorescence spectra of many biomolecules overlap.
isomers. The case of molecular isotopes is based on the mass difference between the molecular components which results in a slightly different revival period of excitation degree of the other. In our work we implemented this approach to molecular nitrogen, and study the cases of molecular isotopes and molecular spin using ultrashort laser pulses where the first pulse rotationally excites both components in a binary mixture, and the second pulse de-excites one, while enhancing the other. 

We experimentally demonstrate a new approach to selective excitation of close molecular species in mixtures. We apply two time delayed, YEHIAM PRIOR, SHARLY FLEISCHER, ILYA SH. AVERBUKH, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, and isomers diffusion-space pattern helps indicate the area in the search space that is most amenable to effective optimization. The diffusion-mapping algorithm is sufficiently effective in maximizing integrated intensity in a second harmonic generation experiment. The use of a sampling set of 1000 random pulses in the diffusion mapping detection space and to sample essential patterns in the lower-dimensional representation. The diffusion maps are constructed and analyzed for the case study here, we use the recently developed nonlinear statistical method of diffusion mapping to effectively reduce the combined dimensionality of the search and detection spaces are high-dimensional (with dimension $\sim$100 each). This poses considerable problems to analysis and interpretation of the process-related data. 

Photonics Research, Temple University, Philadelphia, PA 19122 — Strong-field control settings involve highly nonlinear processes. Typically, both search and detection spaces are high-dimensional (with dimension $\sim$100 each). This poses considerable problems to analysis and interpretation of the process-related data. 

Here, we use the recently developed nonlinear statistical method of diffusion mapping to effectively reduce the combined dimensionality of the search and detection space and to sample essential patterns in the lower-dimensional representation. The diffusion maps are constructed and analyzed for the case study of maximizing integrated intensity in a second harmonic generation experiment. The use of a sampling set of 1000 random pulses in the diffusion mapping detection space is sufficient for effective dimensionality reduction and for revealing the inherent structure of the process-related data. Extrapolation of the low-dimensional diffusion-space pattern helps indicate the area in the search space that is most amenable to effective optimization. The diffusion-mapping algorithm is sufficiently fast and robust that may make it a valuable preprocessing tool for optimal pulse searching.

Selective Rotational Manipulations of Close Molecular Species – isotopes and isomers, YEHIAM PRIOR, SHARLY FLEISCHER, ILYA SH. AVERBUKH, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — We experimentally demonstrate a new approach to selective excitation of close molecular species in mixtures. We apply two time delay, ultrashort laser pulses where the first pulse rotationally excites both components in a binary mixture, and the second pulse de-excites one, while enhancing the excitation degree of the other. In our work we implemented this approach to molecular nitrogen, and study the cases of molecular isotopes and molecular spin isomers. The case of molecular isotopes is based on the mass difference between the molecular components which results in a slightly different revival period of the repetitive alignment that follows excitation by an ultrashort pulse. Following the revival process, one can distinguish between the isotopic components and selectively affect them. The case of spin isomers is more complicated since there are no differences in their mechanical or electrical properties. Here we utilize the symmetry and statistics of the specific molecular wavefunction and demonstrate highly selective ($\sim$18:1) excitation of Ortho/Para nitrogen. Numerical simulations agree very well with the observed results. Since this process is nonresonant and does not require any special conditions like temperature etc. this approach is general and can be applied to most symmetric molecules. 

Anti-Correlated Pigment Fluctuations of Allophycocyanin for Highly Efficient Photosynthetic Light Harvesting in Cyanobacteria, ANDREW MORAN, University of North Carolina, RENE NOME, NORBERT SCHERER, University of Chicago — The phycobiliprotein, allophycocyanin (APC), is an excellent model system for the study of light harvesting pigment interactions with a protein bath. This work investigates the relaxation of electronic excitations in APC with electric field–resolved transient grating and photon echo spectroscopies. Transient grating experiments observe a 35 fs internal conversion process between single exciton levels. Most importantly, our analysis shows that anti-correlated phycocyanobilin pigment energy level fluctuations cause the anti-diagonal orientation of the node in the measured dispersive photon echo spectrum. We believe this novel observation to reflect concerted protein bath fluctuations over the 2 nm length scale that separates the pigments. Consideration of the Forster energy transfer rate theory suggests that APC has evolved with this property to enhance its photosynthetic light harvesting efficiency. 

10:24AM P26.00007 ABSTRACT WITHDRAWN – 

Understanding the relaxation of excited-state cis-1,3,5-hexatriene in order to augment the preferred pathway for control, MICHAEL ORROZCO, KUO-CHUN TANG, ROSEANNE SENSION, Dept. of Chem., University of Michigan - Ann Arbor — A study of the ground and excited-state relaxation of cis-1,3,5-hexatriene in various solvents and temperatures has been performed. The role solvent plays in the relaxation dynamics and relaxation pathways has been assessed and modeled to achieve a better understanding of the energy landscape. This information will be used to determine the preferred relaxation pathways and inform efforts to use sculpted UV pulses to influence the excited state dynamics through pump-dump interactions. Finally, further experiments are proposed wherein UV pulse-shaping will used to study and control other reactive systems.
8:00AM P27.00001 Magnetic Stripe Phase at the Spin Reorientation Transition of an Ultrathin Magnetic Film†. Y.Z. WU, Surface Physics Laboratory (National Key Laboratory) and Advanced Material Laboratory, Fudan University, Shanghai 200433, China — Magnetic long-range order cannot exist in an isotropic 2D Heisenberg system at any finite temperature, but could be established by adding a magnetic anisotropy to the system. In experiment, this topic has been addressed by investigating the so-called spin reorientation transition (SRT) in magnetic ultra-thin films, where the perpendicular magneto-crystalline anisotropy cancels the in-plane magnetic shape anisotropy. In this talk, we present our study on the SRT of Fe/Ni/Cu(100) system using Photoemission Electron Microscopy (PSEM) chamber at beam line 7.3.1.1 of the Advanced Light Source. We show that (1) a homogenous magnetic state is energetically unstable against the formation of magnetic stripe domains, (2) the stripe domain width decreases exponentially towards the SRT point, and (3) the Curie temperature of the film is reduced to result in a paramagnetic phase within a narrow thickness gap in the SRT region. Using magnetic interlayer coupling to simulate the effect of an external magnetic field, we further studied the SRT in Co/Cu/(Fe/Ni)/Cu(100) system and revealed a universal behavior of the stripe domain width. Moreover a new metastable bubble domain phase was observed near the SRT point in Fe/Ni film, which enriches the magnetic phase diagram of a 2D magnetic system.

†Work was done in collaboration with C. Won, J. Choi, J. Wu, A. Doran, A. Scholl, and Z. Q. Qiu.

8:36AM P27.00002 Induced V magnetic polarization effects in V/Fe/V trilayers. ROSA A. LUKASZEW, CESAR CLAVERO, College of William and Mary, YONGSEONG CHOI, DANIEL HASKEL, APS-ANL, CECILIA SANCHEZ-HANKE, NSLS-BNL, BRIAN KIRBY, NIST, MIKE FITZSIMMONS, LANSCE-LANL — Understanding magnetic interactions at interfaces between nonmagnetic and magnetic elements and in some cases magnetic polarization of non-magnetic elements at these interfaces is a challenging topic. In addition these phenomena are interesting also due to their potential application in magneto-optical (MO) data storage devices and sensors. In the case of Fe/V interfaces, a fundamental question is the effect of interdiffusion on the magnetic moments of the intervening elements at the interface. Here, we present a structural, morphological and magnetic study of a V/Fe/V trilayer. While no significant diffusion of V into the Fe film was observed with x-ray reflectometry (XRR) and polarized neutrions reflectometry (PNR), x-ray magnetic circular dichroism (XMCD) and x ray resonant magnetic scattering (XMRSS) measurements reveal V magnetic polarization at both Fe/V interfaces. The magnetization profile in the Fe and V films was obtained by XRRMS and will be compared with that obtained with PNR. Our results show the complementarity of these techniques to further clarify V polarization phenomena in Fe/V interfaces.

8:48AM P27.00003 Structure and magnetism of Ni50Mn50 monolayers on Cu3Au(001). WALDEMAR MACEDO, REINALDO OLIVEIRA JR., MAXIMILIANO MARTINS, MANOEL PIRES, CDTN — The growth, structure and magnetism of equiatomic NiMn ultrathin films on Cu3Au(100) and the magnetism of Fe/Femn bilayers on this substrate were investigated. NiMn alloys in a concentration range around 50-50% have an L11 structure with lattice constants a and c of 3.74 Å and 3.52 Å, respectively. This NiMn-phase is antiferromagnetic (AFM), with high Néel temperature (∼1070 K), being very interesting for ferromagnetic / antiferromagnet systems with exchange bias effect and, therefore, for magneto-electronic devices. Cu3Au is an ordered fcc phase with lattice parameter of 3.75 Å, a substrate with very good epitaxial relationship with L11 NiMn. The NiMn monolayers were grown by coevaporation, under molecular beam epitaxy conditions, and characterized in situ by RHEED, LEED, XPS, AES and MOKE. Structural analysis revealed the epitaxy and layer-by-layer growth at room temperature. MOKE measurements suggest that the Fe/Ni50Mn50 bilayers present exchange bias, indicating that equiatomic NiMn films, as grown on Cu3Au(100) at room temperature, is AFM, as expected for the L11.

†Financial support: CNPq, CAPES and CNPq/Millenium Institute of Nanotechnology

9:00AM P27.00004 Ab-initio simulation of magnetic exchange force microscopy of the antiferromagnetic Fe monolayer on W(001). CESAR LAZO, STEFAN HEINZE, Institute of Applied Physics, University of Hamburg, Germany, VASILE CACIUC, HENDRIK HOELSCHER, Institute of Physics, University of Muenster, Germany — Magnetic exchange force microscopy (MexFM) is a promising new technique to perform magnetic imaging with atomic resolution by measuring the magnetic exchange force between a magnetically coated tip and a magnetic sample [1]. Here, we apply density functional theory using the full-potential linearized augmented plane wave (FP-LAPW) method to investigate the exchange forces on the antiferromagnetic monolayer Fe on W(001) [2]. We use an Fe cluster as a tip model and include relaxations of the cluster and the surface. Surprisingly, relaxation effects of tip and sample depend sensitively on the local magnetic configuration. Therefore, relaxations play a crucial role for the magnetic signal. In particular, the onset of the exchange forces is shifted to larger distances, which facilitates their experimental observation. Based on the calculated force-distance curves we simulate MexFM images which display a competition of chemical and magnetic forces. Our simulations can explain the experimentally observed magnetic contrast [3]. [1] U. Kaiser et al., Nature 446, 522 (2007). [2] A. Kubetzka et al., Phys. Rev. Lett. 94, 087204 (2005). [3] R. Schmidt, C. Lazo, et al., submitted (2007).

9:12AM P27.00005 First-principles calculation of low-dimensional magnetic structures†. RUQIAN WU, University of California, Irvine — Magnetism in low dimensions is of great interest for fundamental and industrial research. Density functional calculations are important to provide clear physical insights for search, design and optimization of magnetic nanostructures that are essential in new technologies. We have recently performed systematic studies for search of giant magnetic anisotropy energies in single atom such as 3d on CuN, monatomic wires encompassing 3d-5d atoms, magnetic thin films such as 3d on Cu and Au. We will review the physics that governs the magnetic anisotropy and other phenomena driven by spin-orbit coupling. We will also discuss our recent results of spin dynamics in nanoentities.

†Work was supported by the DOE (grant No: DE-FG02-05ER46237).

9:48AM P27.00006 Shape Anisotropy and Magnetization Modulation in Hexagonal Cobalt Nanowires. ZUWEI LIU, PAICHUN CHANG, CHIA CHI CHANG, G E R D BERGMANN, JIA G. LU, University of Southern California — Ferromagnetic Co nanowires with diameter around 90 nm are synthesized via low voltage electrodeposition method. High resolution transmission electron microscopy and x-ray diffraction results show that the nanowires are uniform in size, and consist predominantly fcc structure with the magnetocrystalline easy axis (-axis) perpendicular to the wire axis. SQUID measurement illustrates the dominance of shape anisotropy, manifested by the weak temperature dependence of the enhanced coercive field along the nanowire axis. The magnetic domain structures of individual, segmented or multiple nanowires are studied via magnetic force microscopy. It shows a strong dipole at the two ends of the nanowire, together with a spatial magnetization modulation along the nanowire with a period around 700 nm. Based on theoretical modeling, such intrinsic modulation originates from the competition between the magnetocrystalline polarization along the easy axis and the shape anisotropy along the nanowire axis.
10:00AM P27.00007 Unique playground for complex magnetism: Fe monolayers on hexagonal transition-metal surfaces, STEFAN HEINZE, JOERG HARDRAT, PAOLO FERRIANI, Institute of Applied Physics, University of Hamburg, Germany, ALI AL-ZUBI, GUSTAV BIHLMAIER, STEFAN BLIEGEL, Institut fuer Festkuerperforschung, Forschungszentrum Juelich, Germany — Recently, the complexity of magnetic order even in single monolayer (ML) thick magnetic films on non-magnetic substrates has been dramatically demonstrated by the discovery of a spin-spiral state for a Mn ML on W(110) [1] and a nanoscale magnetic structure for an Fe ML on Ir(111) [2]. Here, we use density functional theory calculations based on the full-potential linearized augmented plane wave method to systematically study the magnetic order of an Fe ML on hexagonal hcp (0001) and fcc (111) surfaces of 3d- and 5d-transition metals. We show that due to substrate d-band filling the exchange coupling changes gradually from antiferromagnetic (AFM) on Tc, Ru, Re, and Os to ferromagnetic (FM) on Rh, Ir, Pd, and Pt. On Ru and Re the AFM coupling leads to a non-collinear Néel ground state due to topological frustration of exchange interaction. On Ru, Rh and Ir, the nearest-neighbor exchange coupling is small and exchange beyond nearest-neighbors, higher order spin interactions, and anisotropic exchange interaction compete making these systems a playground for intriguing magnetic order. [1] M. Bode et al., Nature 447, 190 (2007). [2] K. von Bergmann et al., PRL 96, 167203 (2006).

10:12AM P27.00008 Mean Field aspects of magnetic domain pattern evolution in ultrathin Fe/Cu(001) films, DANIO PESCIA, ALESSANDRO VINDIGNI, NICULIN SARATZ, OLIVER PORTMANN, Laboratory for Solid State Physics, ETH Zurich, PAOLO POLITI, Istituto dei Sistemi Complessi, CNR Firenze — Ultrathin Fe/Cu(001) films are magnetized out of plane and represent an experimental counterpart of the 2D Dipolar Frustrated Ising Ferromagnet. Indeed, one of the most attractive feature of these films is the occurrence of a variety of magnetic domain patterns; the last few consist of superstructures of positive and negative magnetization which originate from the competition between long-ranged antiferromagnetic dipolar interaction and nearest-neighbor ferromagnetic exchange interaction. The experimental patterns are relatively free to change their characteristic length of modulation as well as their overall structure (striped, labyrinthine, etc.) when the temperature is varied. The Mean Field theory is able to reproduce the temperature dependence of some important experimental observables like the domain width and the inside-domain magnetization profile (obtained by SEMPA images). We report on some Mean Field predictions for the 2D Dipolar Frustrated Ising Ferromagnet in close relationship with quantitative analysis of experimental SEMPA images recorded on Fe/Cu(001) films.

10:24AM P27.00009 Novel magnetism in gold and silver nanoclusters, WEIDONG LUO, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — Ferromagnetic (FM) ordering in transition-metal systems (solids, surface layers, nanoparticles) arises from partially filled d shells. Thus, recent observations of FM Au nanoclusters were unexpected, and an explanation has remained elusive. We report first-principles density-functional spin-polarized calculations for Au and Ag nanoclusters. We find that in highly symmetric Au nanoclusters, the highest-occupied molecular orbital (HOMO) is highly degenerate and partially filled by Au 6s electrons with spins aligned according to Hund’s rule. The nanoclusters behave like “superatoms,” with the spin-aligned electrons being itinerant on the outer shell of atoms. Similar results obtain for Ag nanoclusters. In contrast, the same kind of calculations for Pt nanoclusters find that FM ordering is controlled by the partially filled d states in the usual way, and spin polarization generally occurs in many eigenstates of the Pt clusters. This research was sponsored in part by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and by the McMinn Endowment at Vanderbilt University. Computations were performed at the National Energy Research Scientific Computing Center.

10:36AM P27.00010 Non-Arrhenius Ferromagnetism In 1D Systems, LUCA SPADAFFORA, FAUSTO BORGONI, Dipartimento di Matematica e Fisica, Universita Cattolica, via Musei 41, 25121, Brescia, Italy, LUCA CELARDO, Department of Physics, Tulane University, New Orleans, LA 70118, BRUNO GONCALVES, Emory University, Atlanta, GA 30322 — Topological phase space disconnection has been recently found to be a general phenomenon in isolated anisotropic spin systems. This phenomenon sets a general framework to understand the emergence of ferromagnetism in finite magnetic systems. Here we study its relevance for finite systems in contact with a heat bath. The existence of this threshold, inducing extremely large magnetic reversal times, is shown to be able to determine metastable ferromagnetic behavior in finite samples. Also, it acts as a real energy barrier. Under suitable conditions the law for average reversal times can be obtained analytically and confirmed numerically. Consistent differences from the expected Arrhenius law of reversal times are shown for short rate interacting spin systems.

10:48AM P27.00011 Spin-orbit induced spin-spin coupling between electrons in coupled quantum dots, JIANMIN SUN, SUHAS GANGADHARIAH, OLEG STARYKH, University of Utah — We investigate spin-spin interaction between electrons localized in spatially separated quantum dots. We show that in the presence of single electron spin-orbit interaction (of Rashba type) in the dots and Coulomb interactions between electrons, a new anisotropic coupling of the van der Waals type between spins emerges. Unlike the standard exchange this coupling does not require overlap of the wavefunctions, and as a result becomes dominant for large distance between the dots. This ferromagnetic interaction is important in the Wigner crystal state where the exchange processes are severely suppressed.

Wednesday, March 12, 2008 8:00AM - 11:00AM – Session P28 DCMP: Superlattices and Nanostructures (Wires, Dots, etc.): Optical Properties

8:00AM P28.00001 Enhancement of optical sensitivity of quantum dots near metal-dielectric interface, PRABATH HEWAGEEGANA, VADYM APALKOV — We study theoretically the enhancement of the incident light transmitted through the diffraction grating. We are interested in the mid-infrared frequency range, corresponding to the intraband absorption by quantum dots. We show that for the s-polarized light the enhancement is much stronger than for p-polarized light. By tuning the parameters of the diffraction grating the enhancement of the light can be increased by a few orders of magnitude. The distribution of the transmitted light is highly nonuniform with very sharp peaks with the spatial width about 10 nm. Due to strongly inhomogeneous distribution of electromagnetic field the quantum dots should be placed at special points, i.e. hot spots, with large intensity of the field. We discuss the application of this effect to the quantum dot infrared photodetectors.

8:12AM P28.00002 Surface Enhanced Infrared Absorption Spectroscopy (SEIRA) using Infrared resonant Au-nanoshell based substrates, JANARDAN KUNDU, HUI WANG, Department of Chemistry, Laboratory for Nanophotonics, FEI LE, PETER NORDLANDER, Laboratory for Nanophotonics, Department of Physics and Astronomy, NAOMI HALAS, Department of Chemistry, Laboratory for Nanophotonics, Department of Electrical and Computer Engineering — Enhancements of the molecular signals are known to occur in the mid-IR region when the molecules are in close proximity to rough metal surfaces. This phenomenon, known as surface enhanced infrared absorption (SEIRA), is complementary to surface enhanced Raman scattering (SERS) and can be used for biochemical sensing. However, designing substrates for SEIRA that are resonant in the mid-IR has proven challenging. One solution is to use metal nanoshells, plasmonic nanoparticles with a wide plasmon tunability range from the visible to the mid-IR. Here, we exploit this tunability property of nanoshells to fabricate nanoshell aggregates and nanoshell arrays as SEIRA substrates. Para-aminophenol (pMA) is used as a test molecule for studying SEIRA activity of these substrates. SEIRA enhancement factors are evaluated to be in the 10000 range for these substrates. These strong enhancements allow for sensing of biologically relevant molecules such as adenosine. Spectral interpretation using SEIRA surface selection rule allows for insight into the molecule’s preferred orientation on the nanoparticle surface.
8:24 AM P28.00003 Polarization memory of charged excitons in vertically coupled InAs/GaAs quantum dots. SWATI RAMANATHAN, KUSHAL WIJESUNDARA, MAURICIO GARRIDO, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701-2979, USA. MICHAEL SCHEINBER, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA. — Polarized photoluminescence of the InAs/GaAs coupled quantum dot system was studied, and circular polarization memory signatures of the neutral exciton, the positive trion and the negative trion are reported. Our samples are Stranski-Krastanow dots, vertically separated by a GaAs barrier. We obtain results for circular polarization memory that are consistent with previous polarization studies on single quantum dots, indicating that coupled dot systems have polarization signatures very similar to single dot systems. Due to their structure, our samples display hole level anticrossings. As the system shifts from one positive trion configuration to the other, a continuous change in circular polarization memory is observed. This change in polarization memory is explained by hole tunneling and exchange interactions. Identifying the two positive trion configurations as neutral exciton-like and positive trion-like provides a theoretical basis for understanding the circular polarization memory signature.

8:36 AM P28.00004 Spin interactions in a coupled InAs/GaAs quantum dot studied by polarization dependent photoluminescence. KUSHAL C. WIJESUNDARA, MAURICIO GARRIDO, SWATI RAMANATHAN, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701. MICHAEL SCHEINBER, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375. — In a quantum dot molecule, excitons and trions are relatively long-lived states that can be studied by optical spectroscopy and spin-resolved measurements. Recent experiments on InAs/GaAs quantum dot systems have demonstrated the feasibility of these approaches, and have revealed interesting physics. In this paper, we report on spin-resolved measurements on InAs/GaAs quantum dot systems, and discuss the implications of these results for the development of quantum dot devices.

8:48 AM P28.00005 THz Charge Oscillations in a Modulation Doped Parabolic Quantum Well. JAMES HEYMAN, LAURA BELL, JEFFERY ROGERS, Macla...
9:48AM P28.00010 Coherent coupling and energy transfer enhancement via multi-exciton levels in semiconductor nanocrystals, AMEENAH AL-AHMADI, Department of Physics, Umm Al-Qura University, SA, SERGIO ULLOA, Department of Physics and Astronomy, Ohio University, Athens, OH — The theory of coherent energy transfer (ET) in nanocrystal (NC) systems [1] is generalized for multie exciton levels. The relevant excitonic states in an isolated NC can be described by an effective four-level system, consisting of the ground level, two degenerate single exciton levels, and the biexciton level. We study the dynamics of a single donor-acceptor pair via the equation of motion for the density matrix of the system and consider analytical limits as well as numerical solutions. We show that the enhancement of the ET efficiency introduced by the biexciton levels is limited due to the coherent coupling of the exciton-biexciton levels in the donor-acceptor pair. The saturation of the ET rate in the donor-acceptor pair suggests a new mechanism to control the dipole-dipole coupling strength in NC systems, and we present here its dependence on structure parameters.


10:00AM P28.00011 Luminescence excitation of InAs/GaAs coupled quantum dots, MAURICIO GARRIDO, KUSHAL C. WIJESUNDARA, SWATI RAMANATHAN, ERIC A. STINIAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701, MICHAEL SCHEIBNER, ALLAN S. BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375 — An understanding of the excited states in coupled quantum dots is a necessary step in the road towards a coherent control of this system. Photoluminescence excitation studies were performed on an InAs/GaAs coupled quantum dot system embedded in a Schottky diode structure. The ground states of the positive trion, negative trion and neutral exciton are first clearly identified by their photoluminescence spectra in bias maps. Preliminary results are reported on the luminescence excitation spectra of these charge configurations; both near and far away from the region where molecule-like behavior is observed.

10:12AM P28.00012 Record Extinction of a Laser Beam by a Single Quantum Dot, NICK VAMIVAKAS, METE ATATURE, University of Cambridge, JAN DREISER, TUNC YILMAZ, ANTONIO BADOLATO, Swiss Federal Institute - Zurich, ANNA SWAN, BENNETT GOLDBERG, Boston University, ATAC IMAMOGLU, Swiss Federal Institute - Zurich, SELIM UNLU, Boston University — The ability to efficiently couple far-field light to subwavelength light emitters is of critical importance for the rapidly growing field of nanophotonics. In this talk we present our recent work on the use of both index matched GaAs solid immersion lenses (SIL) and numerical aperture increasing lenses (NAIL) to improve far-field light coupling to and from single InAs/GaAs quantum dots. By incorporating a SIL\NAIL in resonant scattering measurements we find that a single InAs QD can extinguish nearly 12% of the exciting laser beam; a seven-fold improvement in extinction when compared to measurements made without a SIL\NAIL. The strong extinction makes it possible to measure a typical QD extinction using a dc power-meter without the need for phase sensitive lock-in detection.

10:24AM P28.00013 Quantum-mechanical description of Faraday rotation in a single quantum dot, YANJUN MA, JEREMY LEVY — Faraday rotation is one way to realize quantum non-demolition (QND) measurement of electron spin in a quantum dot. In the literature, it has been semiclassically modeled based on quantized electron spin states and classical electromagnetic fields. We have developed a fully quantum- mechanical model to describe Faraday rotation in single quantum dots, using an extension of the Jaynes-Cumming model which includes quantum Stokes operators. The intrinsic noise of Faraday rotation that results from the interaction between photon and electron is quantified under this model. Some effects, such as hyperfine interactions and transitions between off-resonant states such as light hole and conduction band electron states, and have not been included in our calculation. It is believed that these effects will affect the dynamics of spin and based on the current model, our calculation could be extended to examine the behavior of Faraday rotation with these effects included. This work was supported by NSF-DMR-0802846.

10:36AM P28.00014 Optical Aharonov-Bohm oscillations in DMS type-II ZnMnTe/ZnSe quantum dots, I.R. SELLERS, V.R. WHITESIDE, M. EGINLIGIL, University at Buffalo, W.-C. CHOU, National Chiao Tung University, China, I. KHAN, A. PETROU, University at Buffalo, A.O. GOVOROV, Ohio University, B.D. MCCOMBE, University at Buffalo — Low temperature magneto-photo luminescence studies of diluted magnetic semiconductor Zn(Mn)Te quantum dots (QDs) will be presented. As expected, the exchange interaction between the Mn spin and the electric charge carriers results in a strong optical polarization of the luminescence at low temperature. However, in addition, the sample geometry for the structure, which consists of five Zn(Mn)Te QD layers separated by narrow ZnSe spacer layers, will be shown to be particularly suitable for the observation of the optical Aharonov-Bohm effect. This is illustrated by the presence of strong Aharonov-Bohm oscillations in the photoluminescence intensity. Finally, although the (ZnMn)Te system is known to be paramagnetic, at low temperatures the QD structures described display evidence of spontaneous magnetization at zero applied magnetic field both in the optical circular polarization degree and the magnetization. The origin of this behavior will be discussed.

1 This work is supported in part by CSEQuin UB and NSF #EC0524403.

10:48AM P28.00015 Robust Aharonov-Bohm oscillations at elevated temperatures in type-II ZnTe/ZnSe quantum dots, V.R. WHITESIDE, I.R. SELLERS, University at Buffalo, I.L. KUSKOVSKY, Queens College CUNY, A.O. GOVOROV, Ohio University, B.D. MCCOMBE, University at Buffalo — The ZnTe/ZnSe material system is remarkable in that it is possible to study both Te-bound isoelectronic excitons and type-II ZnTe quantum dots (QDs) in the same sample. This is possible since with increasing tellurium deposition there is a clustering of the Te-atoms resulting in an evolution of Te isoelectronic centers, formed by Te-Se substitution, into ZnTe QD structures. The formation of columns of such QDs in multilayer superlattice structures has recently been shown to be particularly suitable for the observation of the optical Aharonov-Bohm effect. Here we present magneto-photo luminescence from such type-II ZnTe/ZnSe QDs that demonstrate large and persistent oscillations in both the exciton energy and intensity at high temperature indicating the formation of coherently rotating states. Furthermore, this high temperature Aharonov-Bohm effect is remarkably robust persisting until 180K despite significant quenching of the luminescence due to ionization of the type-II excitons.

3 This work is supported in part by CSEQuin (UB) and DOE #DEFGO2-05ER46219.

Wednesday, March 12, 2008 8:00AM - 10:48AM — Session P29 DMP: Focus Session: Carbon Nanotubes and Related Materials IX: Graphene Electronic Structure Morial Convention Center 221
8:00AM P29.00001 Veselago lens and p-n junctions in graphene.1, VLADIMIR FALKO, Lancaster University — Both monolayer and bilayer graphene are gapless semiconductors. Their electrostatic modulation can be used to generate single and multiple p-n junctions. We have shown [V. Cheianov and V.I. Fal’ko - Phys. Rev. Lett. 97, 226801 (2006)] that p-n junctions in monolayer graphene are transparent for incident electrons. In particular, those electrons approaching the n-p interface in an almost perpendicular direction can cross it without reflection. Moreover, in graphene the transmission of charge through the n-p interface is quite similar to the refraction of electromagnetic waves at the interface where the refractive index inverts sign [J. Pendry - Nature 423, 22 (2003); J. Pendry - Phys. Rev. Lett. 85, 3966 (2000)]. This is because the electron dispersion in the conduction and valence bands in graphene is such that so that, after an electron crosses the n-p interface, from the n- to p-side, its wave vector becomes directed opposite to its velocity. As a result, n-p junctions in graphene possess intriguing and very promising transport properties: a single straight p-n interface can focus electrons [V. Cheianov, V.I. Fal’ko, B.L. Altshuler - Science 315, 1252 (2007)]. This situation is realised in the n-p junction with equal densities of carriers in the n- and p-regions. Also, we have shown that by varying the carrier density in, e.g., p-side of the junction the focus can be smeared into a pair of caustics meeting each other in a cusp, and calculated the characteristic interference pattern of electron waves in the vicinity of the cusp. Using the idea of fine-tuned focusing of electron flow by the p-n interface, we propose to use n-p-n junctions in a bipolar graphene-based transistor to create Veselago lens and focused beam splitters for electrons.

1 I acknowledge support from EPSRC-UK, the Alexander von Humboldt Foundation and hospitality of Hannover University. This work has been started during the MPI Conference “Graphene Week 2006” at the Max-Planck-Institute for Complex Systems in Dresden.

8:36AM P29.00002 Intradband Landau level transitions in monolayer graphene, ZHIGANG JIANG, Columbia University/NHMFL, E.A. HENRIKSEN, Columbia University, L.C. TUNG, NHMFL, M.E. SCHWARTZ, M. TAKITA, Columbia University, Y.-J. WANG, NHMFL, P. KIM, Columbia University, H.L. STORMER, Columbia University/Bell Labs — We study the cyclotron resonance of electrons and holes in monolayer graphene, via infrared transmission measurements in a magnetic field, $B$, up to 18 T. We find that, instead of having a single resonance energy as in a traditional two-dimensional system, a wide range of transitions between different sets of Landau levels (LLs) can be uniquely distinguished in monolayer graphene. We have observed intraband transitions between neighboring LLs up to $n = 7$, where $n$ is the LL index. As expected from the unusual linear dispersion of the low-energy electronic band of monolayer graphene, we show that the corresponding energies of all observed LL transitions are proportional to $\sqrt{B}$. In addition, beyond such a simple linear dispersion, we find that the measured band bending near the charge-neutral Dirac point ($E = 0$) is $\sim 12\%$ larger than that at higher energies. The LL transitions in the electron and hole bands of monolayer graphene show a considerable asymmetric behavior.

9:48AM P29.00003 High Field Magnetoresistance of Graphene at the Dirac Point1, JOSEPH CHECKELSKY, LU LI, N. P. ONG, Princeton University — The longitudinal and Hall resistance of graphene near the charge neutral point have been studied down to low temperature (20 mK) in high magnetic field (20 T). At issue is the nature of the ground state in the vicinity of the Dirac point in high magnetic fields. In samples in which the off-set voltage is small, we observe a highly unusual approach to an insulating state as the field increases. In samples with $\mu > 0.5$ T$^{-1}$ and $V_0 < 3$ V, the resistance at the Dirac point $R_0$ increases divergently to $M$ in fields of 14-20 T at temperatures $T < 2$ K. This divergent behavior is suppressed in samples with large $V_0$. Surprisingly, this rise shows little temperature dependence below 2 K. The acute dependence on magnetic field and accompanying lack of activated behavior with temperature provides evidence for an unusual cross-over or transition to the insulating state. Implications for theoretical models including gapless edge modes and Quantum Hall Ferromagnetism will be discussed in the context of these results.

1 This work is supported by PCCM Institute at Princeton University.

9:00AM P29.00004 Effect of disorder on transport in a graphene p-n junction1, B. I. SHKLOVSKI, UMN, M. M. FOGLER, UCSD, L. I. GLAZMAN, D. S. NOVIKOV, Yale — We evaluate the resistance of a gate-tunable graphene p-n junction, in which the gradient of the carrier density is controlled by the gate voltage. Depending on this gradient and on the density of charged impurities, the junction resistance is suppressed in samples with large $V_0$, $\mu < 0$. For $V_0 > 0$, the resistance at the Dirac point $R_0$ increases divergently to $M$ in fields of 14-20 T at temperatures $T < 2$ K. This divergent behavior is suppressed in samples with large $V_0$. Surprisingly, this rise shows little temperature dependence below 2 K. The acute dependence on magnetic field and accompanying lack of activated behavior with temperature provides evidence for an unusual cross-over or transition to the insulating state. Implications for theoretical models including gapless edge modes and Quantum Hall Ferromagnetism will be discussed in the context of these results.

1 Supported by NSF, ASC UCSD

9:12AM P29.00005 Nonlinear screening and ballistic transport in a graphene p-n junction1, L. MATTHEW ZHANG, M. M. FOGLER, UCSD — Our theoretical work is devoted to a new class of graphene devices: lateral p-n junctions. Such structures have been recently realized experimentally by modulating the electron density in graphene samples with external gates. We study the charge density distribution, the electric field profile, and the resistance of such p-n junctions. We show that the proper treatment of the electrostatic screening, including nonlinear effects, is crucial for obtaining the correct results for all these quantities. In particular, we show that the total electric field at the interface of the electron and hole regions is strongly enhanced due to limited screening capacity of Dirac quasiparticles. Accordingly, the junction resistance is significantly lower than estimated in previous theoretical literature. At the same time, our new theory enables us to achieve a closer agreement with the recent experiments.

1 Supported by NSF, ASC UCSD

9:24AM P29.00006 Quantum Critical Scaling of Graphene1, DANIEL E. SHEEHY, Louisiana State University, JOERG SCHMALIAN, Ames Lab and Iowa State University — We show that the emergent relativistic symmetry of electrons in graphene near its quantum critical point (QCP) implies a crucial importance of the Coulomb interaction. We derive scaling laws, valid near the QCP, that dictate the nontrivial magnetic and charge response of interacting graphene. Our analysis yields numerous predictions for how the Coulomb interaction will be manifested in experimental observables such as the diamagnetic response and electronic compressibility.

1 This research was supported by the Ames Laboratory, operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.

9:36AM P29.00007 Atomic Collapse and Quasi-Rydberg States in Graphene1, ANDREY SHYTTOV, Brookhaven National Laboratory, LEONID LEVITOV, MIT, MIKHAIL KATSNELSON, Radboud University of Nijmegen — We demonstrate that graphene opens a way to investigate in the laboratory a fundamental quantum relativistic phenomenon, that is, atomic collapse in a strong Coulomb electric field, long-sought for, but still inaccessible in high-energy experiments. We consider charged impurities in graphene and show that an impurity can host an infinite family of Rydberg-like resonance states of massless Dirac particles. Strong coupling of these states to the Dirac continuum via Klein tunneling leads to striking resonance effects with direct signatures in transport and local properties.

1 preprint Arxiv.org:0708.0837
Institute — The dielectric storage (\(\epsilon\) and Conductivity of Multi-Wall Carbon Nanotubes), RAJRATAN BASU, GERMANO IANNACCHIONE, Worcester Polytechnic Center 222.

E conductivity analysis of MWCNT reveals possible mechanisms for how relaxation process (mode-2) is also observed that is independent of 10 branches is fixed by the topological vacuum charge of the insulating BLG state. We discuss how these chiral states can manifest experimentally, and emphasize conventional solitonic zero-modes, their properties are defined by the unusual chiral BLG quasiparticles, from which they derive. The number of zero-mode confinement. These states appear on the domain walls separating insulating regions experiencing the opposite gating polarity. While the states are similar to the measurement). A slow relaxation process (mode-1) is observed that increases in peak frequency with increasing \(E\) but is independent of \(\epsilon\) rot (in-phase and same frequency as the measurement) and \(\epsilon\) rot and shifts to higher frequency with increasing \(E\). A fast downshifts for the G mode and D mode respectively, the softening rate (\(\Delta\omega/\omega\)) is about 1% for both. This behavior is explained by the weakening of carbon-carbon bonds due to elongation, and is consistent with previous studies on carbon nanotubes.

10:12AM P29.00010 Structural and Electronic Properties of Bilayer Epitaxial Graphene, GREGORY M. RUTTER, PHILLIP N. FIRST, Georgia Institute of Technology, Atlanta, GA, JASON N. CRAPIN, JOSEPH A. STROSCIO. Center for Nanoscience and Technology, NIST, Gaithersburg, MD — Scanning tunneling microscopy (STM) and spectroscopy (STS) are used to study the structural and electronic properties of epitaxial graphene on SiC(0001) [1]. We address in this talk the surface morphology and stacking sequence of bilayer graphene. STM topographic images show that in the initial stages of growth, the surface morphology of graphene conforms to an underlying SiC interface reconstruction [1]. In bilayer epitaxial graphene, the top graphene layer forms a continuous sheet across steps separating adjoining terraces. A change in the apparent height between the two graphene basis atoms is observed as a function of tunneling bias. We model the relative heights based on a simple form for the local density of states in AB layer stacking (Bernal, as typical for bulk graphite) [2], and predict a smooth transition from imaging a single sublattice to imaging both sublattices. The experimentally-observed transition is consistent with Bernal stacking of the epitaxial bilayer, and an interlayer hopping energy of 0.4 eV. This work was supported in part by NSF grant ECS-0404084 and Dept. of Commerce/NIST grant 60ANABD6166. [1] G. M. Rutter et al., Science 317, 219 (2007); arXiv:0711.2523. [2] Z. F. Wang et al., Phys. Rev. B 75, 085424 (2007).

10:24AM P29.00011 Aharonov-Bohm effect and broken valley-degeneracy in graphene rings, PATRIK RECHER, U. Leiden, BJØRN TRAUZETTEL, U. Wuerzburg, ADAM RYCEK, U. Jagiellonian, YAROSLAV BLANTER, TU Delft, CARLO BEENAKKER, U. Leiden, ALBERTO MORPURGO, TU Delft — We analyze theoretically the electronic properties of Aharonov-Bohm rings made of graphene. We show that the combined effect of the ring confinement and applied magnetic flux offers a controllable way to lift the orbital degeneracy originating from the two valleys, even in the absence of intervalley scattering. The phenomenon has observable consequences on the persistent current circulating around the closed graphene ring, as well as on the ring conductance. We explicitly confirm this prediction analytically for a circular ring with a smooth boundary modelled by a space-dependent mass term in the Dirac equation. This model describes rings with zero or weak intervalley scattering so that the valley isospin is a good quantum number. The tunable breaking of the valley degeneracy by the flux allows for the controlled manipulation of valley isospins. We compare our analytical model to another type of ring with strong intervalley scattering. For the latter case, we study a ring of polygonal form with lattice-terminated zigzag edges numerically. We find for the hexagonal ring that the orbital degeneracy can still be controlled via the flux, similar to the ring with the mass confinement.

10:36AM P29.00012 Topological configuration in bilayer graphene, IVAR MARTIN, LANL, YAROSLAV BLANTER, ALBERTO MORPURGO, Delft — We study a new type of one-dimensional chiral states that can be created in bilayer graphene (BLG) by electrostatic lateral confinement. These states appear on the domain walls separating insulating regions experiencing the opposite gating polarity. While the states are similar to conventional solitonic zero-modes, their properties are defined by the unusual chiral BLG quasiparticles, from which they derive. The number of zero-mode branches is fixed by the topological vacuum charge of the insulating BLG state. We discuss how these chiral states can manifest experimentally, and emphasize their relevance for valleytronics.

Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P30 DCMP: Electronic Properties of Graphene and Related Structures III Morial Convention Center 222

8:00AM P30.00001 Electric Field and Frequency Dependence of the Dielectric Storage, Loss, and Conductivity of Multi-Wall Carbon Nanotubes, RAJRATAN BASU, GERMANO IANNACCHIONE, Worcester Polytechnic Institute — The dielectric storage (\(\epsilon\)') and loss (\(\epsilon\)'') of the complex dielectric constant (\(\epsilon\)) are reported for multi-wall carbon nanotubes (MWCNT) up to 10^12 Hz as a function of ac-field amplitude E_{rod} (in-phase and same frequency as the measurement) and E_{ac} (fixed phase and frequency with respect to the measurement). A slow relaxation process (mode-1) is observed that increases in peak frequency with increasing E_{rod} but is independent of E_{ac}. A fast relaxation process (mode-2) is also observed that is independent of E_{rod} and shifts to higher frequency with increasing E_{ac} (opposite to that seen for mode-1). A conductivity analysis of MWCNT reveals possible mechanisms for how E_{rod} and E_{ac} can effect the dielectric dissipation differently.

8:12AM P30.00002 The genus g=2 problem- A solution of the Persistent current for the genus g=2 -An application to the Edge currents in Graphene, DAVID SCHMELTZER, CCNY — We report the first solution of Persistent currents for genus g = 2 Aharonov-Bohm coupled rings which form a character “8” structure. For two large coupled rings with equal fluxes, we found that the persistent current in the two coupled rings is equal to that in a single ring. For opposite fluxes the energy has a chaotic structure. This results are obtained within an extension of Dirac’s second class constraints.

1 Collaborative grant CUNY 2007-2008
8:24AM P30.00003 Potential barriers in graphene1, NIMROD STANDER, DAVID GOLDBERGER-GORDON, BENJAMIN HUARD, JOEY SULPIZIO, KATHRYN TODD, BO YANG, Stanford University — Graphene is a single sheet of graphite. Some of its remarkable electronic properties have been predicted over the past 6 decades, but only recently, the Geim group at Manchester succeeded in fabricating graphene and measuring the Quantum Hall effect. These measurements agreed with earlier predictions by observing plateaus at half-integer values and triggered an immense theoretical and experimental effort. It was also predicted that the tunneling through a potential step in graphene is highly anisotropic, and occurs with probability 1 at normal incidence, due to the chiral nature of its quasiparticles. This behavior can be investigated in different potential configurations, such as pn junctions or npm barriers in graphene. In this talk, I will present our experimental work on electronic transport through a tunable potential barrier in top gated graphene devices. I will show that the experiments we have done, depend on the disorder and on the profile of the potential rise across the graphene sheet. Therefore, they can also be seen as a tool to investigate scattering and screening properties in graphene.

8:36AM P30.00004 Effects on the electron conductivity emerging from Majorana zero modes, MIKLOS GULASCI, PASQUALE SODANO, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — The link between single particle random Hamiltonians and non-linear sigma models (NLSM) comes about when setting up a generating function for the mean value taken by the product of Green’s functions. Using the standard machinery of the replica trick we derived disorder averaged product of the retarded and advanced Green’s functions from an effective NLSM describing low energy physics of graphene films with both disorder and defects. We then compute the electron transport properties and we find remarkable effects arising when the defect topology is such that the Majorana fields acquire zero modes.

8:48AM P30.00005 BEC and Superfluidity of Magnetoexcitons in Graphene, OLEG BERMAM, NYC College of Technology of CUNY, GODFREY GUMBS, Hunter College of CUNY — We propose the experimental observation of Bose-Einstein condensation (BEC) and superfluidity of quasi-magnetoexcitons in bilayer graphene. Electrons are in one layer and holes in another which are controlled by an applied gate voltage. We describe the dilute gas of magnetoexcitons with dipole-dipole repulsion in a strong magnetic field $B$ by a $4 \times 4$ matrix Hamiltonian. This Hamiltonian is mapped on to a scalar effective mass Hamiltonian for a dilute gas of dipolar excitons without an applied magnetic field. However, the magnetic field enters through a $B$-dependent effective mass for magnetoexcitons. Moreover, for $N$ excitons, we reduced the problem in a space with $2N \times 2$ dimensions into one with $N \times 2$ dimensions. This is accomplished by integrating over the coordinates of the relative motion of electron and hole. We will present the energy spectrum of collective excitations, the sound spectrum as well as the effective magnetic mass of magnetoexcitons in the strong magnetic field limit. The superfluid density $n_s$ and the temperature of the Kosterlitz-Thouless phase transition $T_c$ are shown to be increasing functions of the excitonic density $n$ and decreasing functions of $B$ and the interlayer separation $d$.

9:00AM P30.00006 Fractionalization in a square-lattice model with time-reversal symmetry1, MARCEL FRANZ, CONAN WEEKS, BABAK SERADJEH, University of British Columbia — We propose a two-dimensional time-reversal invariant system of essentially non-interacting electrons on a square lattice that exhibits configurations with fractional charges ±e/2. These are vortex-like topological defects in the dimerization order parameter describing spatial modulation in the electron hopping amplitudes. Charge fractionalization occurs via a mechanism similar to that in graphene with the “Kekule” distortion and is established by a simple electron counting argument, analytical calculation within the effective low-energy theory, and by an exact numerical diagonalization of the lattice Hamiltonian.

9:12AM P30.00007 Dirac Fermions in a Magnetic Forest1, ANDRES CONCHA, Johns Hopkins University — Recent experimental progress have made it possible to study of a single layer of carbon atoms, i.e. graphene. This newly synthesized material seems to be a promising candidate for building up nano-devices as well as a useful experimental tool to study exotic properties of its low energy excitations. In this work we consider the effect of a vortex lattice in the adjacent superconductor on the transport properties of a graphene sheet. We show that the transport properties of graphene sheets of various geometries can be substantially altered and manipulated by changing the vortex lattice structure and the amount of magnetic flux. A relatively straightforward experimental test of our results is suggested.

9:24AM P30.00008 Phonon-induced many-body renormalization of graphene electronic properties1, WANG-KONG TSE, SANKAR DAS SARMA, University of Maryland — In this talk, we present a many-body theory for the electron-phonon interaction effects on the electronic properties of graphene. We provide analytical results for the electron self-energy, spectral function, and band velocity renormalization due to phonon-mediated electron-electron interaction, showing that phonon-mediated electron-electron coupling has a large effect on the graphene band structure renormalization. Our analytic theory successfully captures the essential features of the observed graphene electron spectra in the angle-resolved photoemission spectroscopy (ARPES) experiments, predicting a kink at $\sim 200$meV below the Fermi level and a reduction of the band velocity by $\sim 10$ – $20\%$ at the experimental doping level.

9:36AM P30.00009 The effect of electronic correlations on Josephson current and proximity effect in SNS graphene junctions, ANNICA BLACK-SCHAFFER, SEBASTIAN DONIACH, Stanford University — Using the self-consistent tight-binding Bogoliubov-de Gennes (BdG) formalism, we investigate the proximity effect and current-phase relationship in SNS graphene Josephson junctions. Both short and long junctions are considered, as well as different doping levels of the graphene. For short junctions at zero doping in the uncorrelated regime our results agree with those found using the non self-consistent Dirac-BdG formalism [1]. We introduce electronic correlations in the Hamiltonian by including the intrinsic nearest-neighbor spin-singlet coupling present in $sp$-bonded planar organic molecules. We study the possibility of coupling this intrinsic $s$- or $d$-wave superconducting pairing [2] to the extrinsic $s$-wave order parameter induced by the metal electrodes. The intrinsic $d$-wave solution, favored in doped graphene, appears for longer doped junctions. For short junctions, the $s$-wave solution can occur, although the result is sensitive to the type of interface. We also report on the two different intrinsic superconducting states’ influence on the supercurrent.

1Supported in part by NSF Grant DMR-0531159

2This work is supported by U.S. ONR.
Density is much weaker in these materials than in conventional porous materials. Our simulations show that this scaling occurs because the nanoscale structure can be used to make porous silica with mechanical properties that remain favorable as the porosity increases. In particular, the elastic modulus scaling with...
8:48AM P31.00003 Phase-field simulations of martensite-martensite nanocomposites 1, MATHIEU BOUVILLE, RAJEEV AHLUWALIA, Institute of Materials Research and Engineering — We study composites made of two martensite-forming materials, with different transition temperatures, $T_1 < T_2$. The system remains austenitic at high temperature, and if the temperature is very low then the difference between the two materials is negligible. We therefore focus on intermediate temperatures, i.e. $T_1 < T < T_2$. Then only one material can transform to martensite — the other transformation may occur only if it is triggered by the martensite already formed (volume changes will then play a key role). We study the effect of reducing the size of the system, in particular how martensite can form in nanocomposites at temperatures at which no martensitic transformation can exist at the macroscopic scale. This work has relevance to multiferroics, where the phase transformation in one material (e.g. ferroelectric) triggers a transformation in another material, for instance magnetostrictive.

9:00AM P31.00004 The dynamical activation-relaxation technique (DART): an on-the-fly kinematic Monte-Carlo algorithm 1, FADWA EL-MELLOUHI, MICHEL COTE, LAURENT J. LEWIS, NORMAND MOUSSEAU, Dep. de physique et RQMP, Univ. de Montreal, Quebec, Canada — We present DART, the dynamical activation-relaxation technique, that combines the activation-relaxation technique (ART) with a non-lattice KMC method that allows the on-the-fly identification of barriers and the full treatment of lattice deformations. Most KMC schemes rely on the use of a fixed list of events and barriers, which are drawn with the proper weight during the simulation. While this works well for a number of problems (such as metal-on-metal growth), it cannot be used for processes where the events may change with time. DART overcomes this limitation. ART nouveau has been used extensively for the study of activated mechanisms in different materials within both an empirical and an ab-initio description of the systems. In the DART implementation, KMC moves are based on a catalog of events constructed on-the-fly using ART. After each KMC move, this catalog is updated so as to take into account new environments that may appear. A topological description of the structure of the system at each moment allows the method to identify rapidly these new environments and to move forward efficiently. In this talk, we will describe the method and present the case of interstitial diffusion in Si. Our results are compared with previous molecular-dynamics and on-lattice KMC simulations.

9:12AM P31.00005 Charge patching method for the calculation of electronic structure of organic semiconductors 1, NENAD VUKMIROVIC, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The electronic structure of organic semiconducting conjugated polymers and molecular crystals is essential in determining their optical and transport properties. Such organic semiconductor systems have potential applications for solar cells, field-effect transistors and luminescent devices. However, for such systems containing a large number of atoms, the direct calculations based on density functional theory (DFT) are often not feasible. Here we present the development of the charge patching method for the calculations of organic systems, a method which was previously successful in treating inorganic semiconductor materials [1]. The results of the calculations for alkane and alkene chains using this approach yield the difference in Kohn-Sham wavefunction eigenenergies of the order of only 30 meV compared with direct DFT calculations. Further investigations involving aromatic compounds, as well as elements such as sulfur, nitrogen, and oxygen, will be presented. [1] L.W. Wang, Phys. Rev. Lett. 88, 256402 (2002).

9:24AM P31.00006 Real-space grid representation of momentum and kinetic energy operators for electronic structure calculations 1, DOMENICO NINNO, GIOVANNI CANTELE, FABIO TRANI, Università di Napoli Federico II, Dip. di Scienza Fisiche, Via Cintia, I-80126, Napoli — The development of computational methods based on real-space grids is contributing to the advances and understanding of nanoscale materials. Real-space grids methods, particularly within the pseudopotential density functional theory, have the advantage of producing highly structured matrices paving the way towards grid-based O(N) methods for both DFT total energy and molecular dynamics calculations. However, a limitation seems to be the lack of a basis set putting these approaches on a different ground with respect to standard methods. We prove that this limitation is only apparent showing that the position operator eigenkets are the natural basis set for the finite difference representation of momentum and kinetic energy operators. Some conceptual points and unpublished results related to the connection between the discrete and the continuum representations will be discussed.

9:36AM P31.00007 Single molecular NDR: A first principles study 1, RANJIT PATI, Department of Physics, Michigan Technological University, Houghton, MI 49931 — The demonstration of single molecule switch with a negative differential resistance (NDR) feature has drawn considerable attention in recent years. The NDR feature is described by a steady increase followed by a decrease in current with the increase in applied bias. Here we report a single molecular NDR in a strongly coupled metal-molecule junction, with peak to valley ratio (PVR) of 2.7 at both positive and negative bias. The bias dependent screening effect is explicitly included in our calculation through a rigorous self-consistent many body approach. The non equilibrium Green function approach is used to calculate the quantum transport. The origin of high PVR will be discussed.

9:48AM P31.00008 Electron correlations in molecular wires: e-e interactionion both in leads and bridge 1, YURI DHANOVSKY, Department of Physics & Astronomy, University of Wyoming, Laramie, WY 82071, VINCE ORTIZ, Department of Chemistry & Biochemistry, Auburn University, Auburn — Molecular systems (molecules) with strong electron-electron interaction both in leads and a bridge are described in terms of the time-dependent electron Green functions. We prove that the Meir-Wingreen expression holds if one assumes that the bridge and lead electron subsystems are strongly separated. We develop a diagrammatic technique in a well determined, noncrossing cluster approximation. Within this approach, Dyson equations for various nonequilibrium Green functions are derived, and the validity conditions are found. In addition, we rigorously prove that despite strong electron-electron or electron-vibration interaction in the systems with the finite number of quantum states, the Landauer-Buttiker expression for electric current is true. The ab initio electron propagator method is applied to the calculations of I-V characteristics in molecular electronic devices with the bridge composed from 1,4-benzene–dithiolate molecule.

1 We acknowledge funding from FQRNT.

1 This work was supported by U.S. Department of Energy and used the resources of National Energy Research Scientific Computing Center.

1 This work is supported by National Science Foundation under grant ECS-0643420.

1 We are grateful to the National Science Foundation that has supported this research through grant CHE-0426090.
10:00AM P31.00009 Characterizing Capture-Zone Distributions: Generalized Wigner vs. Alternative Forms, and Experimental Fits\textsuperscript{1}, T.L. EINSTEIN, ALBERTO PIMPINELLI\textsuperscript{2}, U. of Maryland, College Park — In problems of growth of islands or of dots, it is often advantageous to consider the distribution of the areas of proximity (Voronoi) cells of nucleation sites, i.e. the capture zones (CZ). Extending results for terrace-width distributions on vicinal surfaces\textsuperscript{3} we have shown that the (non-equilibrium, steady-state) CZ distribution is well described by the generalized Wigner expression \( P_b(s) = a^b \exp(-bs^2) \) [with \( a \) and \( b \) being constants assuring normalization and unit mean, and \( s \) here the CZ area divided by its mean], which accounts for a strikingly broad range of fluctuation phenomena. For CZ distributions we find that the single adjustable parameter \( g = (2/d)(i + 1) \), where \( i \) is the size of the critical nucleus and \( d \) (= 1 or 2) the spatial dimensionality\textsuperscript{4}. We emphasize comparisons with other fitting expressions (esp. gamma functions), new applications to experimental data, and the generality of \( P_b(s) \).

\textsuperscript{1}Work at UMd supported by the MRSEC, NSF Grant DMR 05-20471 and partially by DOE CMSN grant DEFG0206ER46227. Visits to UMd by AP supported by CNRS Travel Grant

\textsuperscript{2}Also U. Blaise-Pascal, Clermont-2, Aubière, France

\textsuperscript{3}AP et al., PRL 95, 246101 (2005); TLE, Appl. Phys. A 87, 375 (2007)

\textsuperscript{4}A. Pimpinelli and T.L. Einstein, PRL 99, 226102 (2007).

10:12AM P31.00010 Molecular simulations of capillary adhesion\textsuperscript{1}, SHENGFENG CHENG, MARK ROBBINS, Johns Hopkins University — Adhesion due to capillary condensation is ubiquitous in nature, and dominates the adhesion force between particles in many experiments. Traditional models are based on continuum theory and may not describe nanoscale capillaries in microelectromechanical systems (MEMs) or at an atomic force microscope (AFM) tip. We employ molecular dynamics simulations to investigate the capillary adhesion between a nominally spherical tip and a flat substrate with a liquid bridge of fixed volume. The atomic scale roughness on the tip, contact angle and volume are varied. The adhesive force-distance curve and the separate contributions from Laplace pressure and surface tension are compared to continuum theory using independently measured parameters. Continuum theory provides a good description down to separations of a few molecular diameters. Atomic scale roughness affects the contact angle that enters the continuum theory and alters the adhesive force.

\textsuperscript{1}Work supported by Grants CTS-0320907-DLMS and NIRT-0709187.


10:36AM P31.00012 An algebraic approach to computer program design and memory management\textsuperscript{1}, JAMES RAYNOLDS, University at Albany, State University of New York, LENORE MULLIN, National Science Foundation — Beginning with an algebra of multi-dimensional arrays and following a set of reduction rules embodying a calculus of array indices, we translate (in a mechanizable way) from the high-level mathematics of any array-based problem and a machine specification to a mathematically-optimized implementation. Raynolds and Mullin introduced the name Conformal Computing\textsuperscript{2} to describe this process that will be discussed in the context of data transforms such as the Fast Fourier, Wavelet Transforms and QR decomposition. We discuss the discovery that the access patterns of the Wavelet Transform form a sufficiently regular subset of those for our cache-optimized FFT so that we can be assured of achieving similar efficiency improvements to the Wavelet Transform as those that were found for the FFT. We present recent results in which careful attention to reproducible computational experiments in a dedicated/non-shared environment is demonstrated to be essential in order to optimally measure the response of the system (in this case the computer itself is the object of study) so as to be able to optimally tune the algorithm to the numerous cost functions associated with all of the elements of the memory/disk/network hierarchy. * The name Conformal Computing is protected: © 2003, The Research Foundation, State University of New York.

10:48AM P31.00013 Giant Hall Effect in Laterally Inhomogeneous 2D Electron Gas\textsuperscript{1}, HANG XIE, PING SHENG, Department of Physics, Hong Kong University of Science and Technology — Giant Hall effect has been observed in non-magnetic granular metals at concentration close to the quantum percolation threshold [1], attributable to quantum interference effect. In this work we numerically simulate the Hall effect for 2D electron gas in a laterally inhomogeneous structure. At scales smaller than the electron dephasing length, we obtain the Hall coefficient of 2DEG by solving Schrodinger’s equation, with 4 leads connected to the sample. It is shown that for special (laterally) nano-scaled structures, the Hall coefficient can be enhanced by at least 3 orders of magnitude. We have also simulated the effect of assembling such structures into a macroscopic sample, by solving the Laplace equation.


Wednesday, March 12, 2008 8:00AM - 11:00AM — Session P32 GMAG FIAP: Focus Session: Magnetic Media and Hard Magnetic Materials Morial Convention Center 225
8:00AM P32.00001 Magnetism of FePt nanoparticles and nanodot arrays.1 HAO ZENG, University at Buffalo-SUNY — L10 structured FePt materials show great potential for magnetic data storage media applications.1 The first part of this talk concerns the magnetism in chemically synthesized FePt nanoparticles. Discrete FePt nanoparticles with L10 structure have recently been realized by salt annealing, making it possible to study their size dependent magnetic properties.2 We have discovered a strong reduction of magnetization with decreasing FePt particle size and an unusual temperature dependent magnetization that deviates from the Bloch’s T²/² law at low temperatures. A model based on competing exchange interactions is proposed to explain this unusual behavior, considering explicitly the nanoparticle shape. FePt system has complicated exchange interactions, with interaction in the (100) plane being strongly ferromagnetic and inter-plane much weaker. The ferromagnetic and antiferromagnetic exchange interactions contribute differently at the nanoparticle surface and interior, leading to reduced ferromagnetic order at the surface terminated by facets. The model correctly explains the magnetization reduction with decreasing particle size, a surface paramagnetic phase as evidenced by Mossbauer spectroscopy and the unusual temperature dependent magnetization behavior. The second part of this talk will report our recent efforts in developing ordered FePt nanodot arrays using self-assembled porous templates as evaporation masks. The arrays possess perpendicular anisotropy, large coercivity and extremely high density, all of which are desirable features for future data storage media.

8:36AM P32.00002 Permanent-Magnetic Fe-Pt Nanoparticles1 RALPH SKOMSKI, D.J. SELLMYER, Department of Physics and Astronomy and NCMN, University of Nebraska — Recently, it has become possible to produce magnetically stable small-scale single-phase [1] and hard-soft [2] Fe-Pt nanoparticles with potential applications in permanent magnetism. The coercivity is largely determined by the degree of L10 ordering and the presence of the soft phase, respectively, and affected by surface anisotropy. We model the coercivity of the particles as a function of composition, structure, and particle diameter. The smallest particles reverse coherently, with renormalized anisotropy constants, but with increasing size, micromagnetic correlations become important. The reversal modes in the two-phase particles are reminiscent of p-state wave functions in atomic physics [2] and well described by second-order perturbation theory. We also discuss extensions involving semihard phases, which may be created by substitutions or coatings using heavy transition metals, such as Pt and W. One example is hexagonal Co1−xPtx, which exhibits a huge anisotropy per Pt atom and a substantial net anisotropy. - [1] C. B. Rong et al., Adv. Mater. 18, 2984 (2006). - [2] J. E. Shield et al., JAP 99, 08BS08 (2006). - [3] R. Skomski, Simple Models of Magnetism, University Press, Oxford 2008.

Work supported by DOE and NCMN.

8:48AM P32.00003 FePt Nano-particles and Nano-wires1 LEVENT COLAK, GEORGE HADJIPANAYIS, UNIVERSITY OF DELAWARE TEAM — In this work, we have studied the microstructure and magnetic properties of FePt nano-particles, nano-rods, and nano-wires synthesized by modified chemical synthesis route described elsewhere[1,2]. The effect of synthesis parameters on the particle shape has been investigated for nanoparticles with sizes of 5-7 nm, for nano-rods and nano-wires with a diameter of 2-3 nm and a length of 20 and 100 nm, respectively. Low injection temperature for the iron precursor and usage of surfactants as reaction solvents resulted in 7 nm nano-cubes whereas a high heating rate to refluxing temperature and high injection temperature resulted in spherical shapes with 5 nm diameter. Nano-rods and nano-wires are formed by simply adjusting the relative ratios of surfactants to reaction solvents (oleic acid, oleyl amine and octadecene/benzylether) and the refluxing time. Transmission electron microscope (TEM) studies show that usage of high concentrations of oleyl amine and longer refluxing times induce nano-wire formation. HRTEM and magnetometry studies are currently in progress to investigate the development of morphology and microstructure during the synthesis and determine their influence on the magnetic properties. 1. C. Wang et. al. Angew. Chem. Int. Ed. 2007, 46,1-4. 2. M. Chen et. al. J. Am. Chem. Soc. 2007, 129, 6348-6349.

9:00AM P32.00004 Nanostructure and Magnetic Properties L10 FePt Films with Additions of Au and Cu. T. GEORGE, M. YAN, Y. XU, R. SKOMSKI, R. KIRBY, D. J. SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska — Non-epitaxially grown L10 FePt/Au and FePt/Cu films have been fabricated and investigated. All films are initially deposited with the structure [FePt]/[Au] and have individual layer thicknesses from about 0.1 nm to 1 nm. The L10 phase is achieved by post-deposition annealing at temperatures from 500 to 600 °C for varying times. XRD and TEM show that Cu enters the L10 lattice whereas Au segregates at the grain boundaries. Both types of films exhibit a decrease in M_s due to magnetic dilution. The coercivity (H_c) increases and decreases with the addition of Au and Cu, respectively. These changes are due to reduced anisotropy (Cu) and to reduced inter-granular exchange coupling (Au). In the FePtAu films, MFM shows a decrease in magnetic coherence length (L_M) from 90 to 74 nm and the M – H slope α = (dM/dH)_{sat} decreases from 5.7 to 0.9 for Au contents from zero to 32 vol%. A simple interaction model quantifies these trends by considering that intergranular exchange cooperatively enhances both α and L_M. In the FePtCu films, the addition of Cu yields a decrease in Curie temperature (574 K at 20 vol%). - Work supported by NSF DMR 0302544.

9:12AM P32.00005 Electric field assisted magnetization reversal in FePt films. PAVEL LUKASHEV, University of Nebraska, Omaha, KIRILL BELASHCHENKO, University of Nebraska, Lincoln, RENAT SABIRIANOV, University of Nebraska, Omaha — We propose to use strain assisted reduction in anisotropy of FePt in order to make magnetization reversal easier in the writing of the magnetic storage devices. We performed first-principles calculations of the magnetocrystalline anisotropy of FePt under bi-axial stress using full-potential LAPW implemented in FLEUR code. Magnetocrystalline anisotropy decreases by 25% with application of 1.5% tensile biaxial strain. This is partially due to the reduction of the c/a ratio by about 1.5% (calculated Poisson ratio is 0.33) in the tetragonal cell and partially due to the increase in volume by about 1.5%. Biaxial strain can be obtained by placing piezoelectric film under FePt layer, and by applying electric field on the system. Modern ferroelectric systems can provide stress up to 2%. Besides, we propose using thin ferroelectric films with asymmetric interfaces, which provides a simple way to generate bias field in the polarization reversal and related properties. The existence of the polar interfaces results in a different average polarization in the film upon reversal. As a result, the strain in the film depends on the direction of polarization. This asymmetric strain can be used do modulate magnetic properties.

9:24AM P32.00006 Influence of interfacial non-magnetic materials on soft-hard bilayer interaction. A. ZAMBAHO, H. OGUCHI, J. TAKEUCHI, Univ.of Maryland, S. LOFLAND, Rowan Univ., J. LIU, Univ.of Texas, D. JOSELL, L. BENDERSKY, NIST, Y. LIU, Z. WANG, Georgia Tech — Among the factors that affect this behavior and how the interface nonmagnetic material can significantly alter the nature of the interaction. Such behavior can have a pronounced effect on hard-soft bulk nanocomposite magnets. ONR MURI N00014-05-1-0497.

9:36AM P32.00007 Depth dependence of anisotropy in graded Co/Pd multilayers, S.M. WATSON, J.E. DAVIES, NIST, K. LIU, UC-Davis, G.T. ZIMANYI, B.J. KIRBY, J.A. BORCHERS, NIST — As the magnetic recording industry looks beyond perpendicular recording [1] multilayered media such as exchange coupled composite [2] and graded media [3] have the potential for increasing storage density by combining low and high anisotropy materials. The soft layer reduces the required write field while the hard layer helps to maintain the thermal stability. Recent work has shown further enhancements when the anisotropy is gradually increased up to the hard layer anisotropy [3]. Grading the media in this manner is difficult to do experimentally. Equally difficult is accurately measuring the properties that make these materials unique, namely the depth dependence of the anisotropy. In this study we used polarized neutron reflectometry to measure the in-plane magnetization depth profile of graded Co/Pd multilayers with perpendicular-to-plane easy axis as a function of in-plane applied field. This technique allowed us to observe the depth-dependent response of the spins as they were pulled away from their easy axis, thus allowing us to determine the depth dependence of the anisotropy field. [1] M. Mallary, et al. IEEE Trans. Magn. 38, 1719 (2002). [2] R. Victora, et al. IEEE Trans. Magn. 41, 2828 (2005). [3] D. Suess, Appl. Phys. Lett. 89, 189901 (2006).

9:48AM P32.00008 Fast Reversal in Multilayer Exchange Spring Media, D. SUESS, Vienna University of Technology — Hard disk media that support ultra high densities require small grains in order to obtain high signal to noise ratios. The use of high coercive materials such as alloys in the L10 phase allow for thermally stable grains at grain diameters in the order of 4nm. However state of the art write heads produces too small fields to reverse these extremely hard magnetic grains. Recently composite media and exchange spring wire were proposed in order to decrease the write field requirements [1,2]. In exchange spring media an ultra hard magnetic storage layer is strongly exchange coupled to a softer magnetic nucleation host layer. The nucleation host decreases the switching field of the storage layer up to a factor of five without lowering the thermal stability of the entire structure. If the nucleation host is composed of multiple magnetic layers where the anisotropy increases from layer to layer it was shown that the resulting structure has a high thermal stability whereas at the same time the coercive field decreases with one over the total layer thickness [3]. Besides the previous results which were obtained in the quasi static limit, where the external field was applied slowly (several nanosecond) further surprising effects occur if the field rise time is in the order of several hundred picoseconds. These fast field rise times together with small damping constants in the media allow for precessional switching in composite media. It was demonstrated that precessional switching significantly lowers the coercive field [4] and also leads to ultra fast reversal modes [5]. We will present results on the reversal time of magnetic bilayers and magnetic trilayers in the precessional switching regime. Micromagnetic simulations show that a magnetic bilayer with a total thickness of 25 nm (hard layer anisotropy is $K = 1 \text{ MJ/m}^2$) can be reversed with a field pulse of 20 ps. Interestingly the reversal time increases to 0.5 ns as the field rise time is decreased from 0.1 ns to 0.01 ns.

10:24AM P32.00009 Role of dipolar interactions in the determination of intrinsic switching field distributions in perpendicular recording media1, YANG LIU, KARIN DAHMEN, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA, ANDREAS BERGER, CIC nanoGUNE Consolider, E-20009 Donostia - San Sebastian, Spain — The $\Delta H(M, \Delta M)$ method and its ability to determine the intrinsic switching field distributions of perpendicular recording media are numerically studied with the coupled hysteron model. It is found that the presence of dipolar interactions with strength of practical recording media enhances the reliability of the $\Delta H(f; \Delta M)$ method. The correlation between the fit quality measure and the deviation from redundancy measure indicates that the latter, which can be determined from experimental data alone, is a good predictor of the reliability.


10:36AM P32.00010 Chiral electrical DW injection and single shot detection for ultra-high density data storage, L. O’BRIEN, Imperial College London, D.E. READ, D. PETIT, A.-V. JAUSOVEC, E.R. LEWIS, H.T. ZENG, R.P. COWBURN — Ultra high density data storage devices based on magnetic domain walls (DWs) propagating through Permalloy (Py) nanowires have recently been proposed [Cowburn et al., Science 2005]. Controlling the chirality (defined as the sense of rotation of the magnetic moments within the DW) of the DW is of vital importance for proper functioning of these devices. Chiral DW injection can be achieved using global magnetic fields; however, technological applications require this to be carried out using independent, localised fields in multiple wires simultaneously. Using the Oersted field from pulsed electrical currents passing through gold wires (∼40µm wide, ∼200nm thick) fabricated at an angle over Py nanowires (100nm wide, 10nm thick) we inject transverse DWs. The chirality of the DWs is probed using spatially resolved MOKE measurements of their chirality dependent interaction with a cross-shaped trap. The results are consistent with chirally controlled DW injection. In addition, we are able to individually address four parallel wires and detect DW propagation using single shot MOKE measurements. Electrical readout was separately demonstrated by detecting the presence of single DWs at the end of a wire using Anisotropic Magnetoresistance (AMR) measurements.

10:48AM P32.00011 Effect of Grain size on the Giant Intrinsic Coercivity of High-Energy Milled Sm(Co,Cu,Fe)5 Alloys1, DILARA SULTANA, ALEXANDAR GABAY, GEORGE HADJIPANAYIS, University of Delaware, MAGNETICS LAB, UNIVERSITY OF DELAWARE TEAM — The giant intrinsic coercivity of multilayered Sm(Co,Cu)5 alloys have been known for a long time [1]. Previous studies suggested that this behavior is due to the crystal site disorder [2]. Our previous work has explained that the room-temperature intrinsic coercivity of 37 kOe after low-temperature aging is rather due to the intrinsic change in the Co atomic site occupation [3]. In this study, we investigated the effect of grain refinement through the high energy milling on the intrinsic coercivity of the Sm(Co,Cu,Fe)5 alloys. We have found that grain refinement does not affect the high coercivity of homogenized alloys, but strongly influences the onset of the giant coercivity during low-temperature aging. The microstructures of the samples are examined with TEM. [1] E.A. Nesbitt, R.H. Willens, R.C. Sherwood, E. Buehler, J.H. Wernick 1968 Appl. Phys. Lett. 12, 361. [2] H. Oesterriech, F.T. Parker, M. Misroa 1979 J. Appl. Phys. 50, 4273. [3] A.M. Gabay, P. Larson, I.I. Manzin, G.C. Hadijivanayis 2005, J. Phys. D: Appl. Phys. 38, 1.

1 work supported by DOE

Wednesday, March 12, 2008 8:00AM - 10:48AM
8:00AM P33.00001 Generation, Modulation and Electrical Detection of Spin Currents in Silicon in a Lateral Transport Geometry1. BEREND JONKER, Naval Research Laboratory — The electron’s spin angular momentum is one of several alternative state variables under consideration on the International Technology Roadmap for Semiconductors. Electrical injection / transport of spin-polarized carriers is a prerequisite for developing such an approach. While significant progress has been realized in GaAs, little has been made in Si. Electrical injection of spin-polarized electrons is demonstrated in Fe/AlO3/Si (001) n-i-p structures by using the circular polarization of the electroluminescence (EL). The EL polarization tracks the Fe magnetization, confirming spin injection into the Si, and reflects Fe majority spin, consistent with the common delta-symmetry of the Fe and Si bands. The Si spin polarization is \( \sim \)30% at 5K, with significant polarization extending to at least 125K. These results are confirmed in Fe/AlO3/Si/AlGaAs/GaAs quantum well structures – the GaAs EL shows that spin transport occurs despite poor crystalline quality of Si epi-layers on GaAs, the 0.3 eV Si/AlGaAs CB offset, and air exposure of the interfaces. Lateral transport structures and non-local detection techniques are used to create a spin current which flows separately from the spin-polarized charge current. This spin diffusion current is sensitive to the relative magnetizations of the injecting and detecting contacts, and can be modulated by a perpendicular magnetic field (Hanle effect) which causes precession in the transport channel. The generation of spin currents, coherent spin precession and electrical detection using magnetic tunnel barrier contacts and a simple lateral device geometry compatible with “back-end” Si processing will facilitate development of Si-based spintronic devices.


1This work was supported by ONR and core programs at NRL.

8:36AM P33.00002 Electrical Spin injection into Silicon: a comparison between Fe/Schottky and Fe/AlO3 tunnel contacts. G. KIOSEOGLOU, A.T. HANBICKI, C.H. LI, P.E. THOMPSON, R. GOSWAMI, G. SPANOS, B.T. JONKER, Naval Research Laboratory — We have recently demonstrated successful electrical injection of spin-polarized electrons from an Fe film through an AlO3 tunnel barrier into Si [1]. The spin polarization in the Si is \( \sim \)30% at 5K, with significant polarization sustained to at least 125K. In this study we compare electrical spin injection from Fe into Si, using vertical device structures, with spin injection from Fe into Si using lateral structures by reverse biased Fe/Si Schottky contact and a Fe/AlO3 tunnel barrier. For both types of structures the electroluminescence (EL) spectra are dominated by transverse acoustic and optical phonon emissions in the Si. The emitted clear circular polarization of the EL due to radiative recombination in the Si tracks the Fe magnetization, confirming that the spin-polarized electrons originate from the Fe for both types of samples. However, the polarization is lower for the Fe/Si contact than that of the Fe/AlO3/Si system. Systematic TEM analysis has been performed to correlate the interface structure with the observed optical polarization, and reveals some Fe/Si intermixing which is absent in the Fe/AlO3/Si structure. [1] B.T. Jonker et al., Nature Physics 3, 542 (2007). This work was supported by ONR and core programs at NRL.

8:48AM P33.00003 Spin transport through n-type doped silicon using electrical methods1, H.-JAE JANG, BIQIN HUANG, IAN APPELBAUM, University of Delaware — In this presentation, we report on all-electrical injection, transport, and detection of spin-polarized electrons through a 3um n-type Phosphorus-doped single-crystal silicon device. Using our hot-electron methods, we demonstrate both spin-valve behavior in an in-plane magnetic field and spin precession in a perpendicular magnetic field. Voltage spectroscopy reveals the effects of charge screening and band bending in the spin transport layer which are not evident in the operation of our previously-studied undoped silicon devices [1,2].

References:

1The authors acknowledge support from DARPA/MTO and the Office of Naval Research.

9:00AM P33.00004 Electrical injection and detection of spin-polarized carriers in silicon in a lateral transport geometry 1. OLAF VAN ’T ERVE, AUBREY HANBICKI, MICHAEL HOLUB, CONNIE LI, CHAFFRA AWO-AFFOUA, PHILIP THOMPSON, BEREND JONKER, Naval Research Laboratory — Significant progress has recently been made on spin injection into the technologically important semiconductors Si and GaAs through lateral heterostructures using different tunnel barriers- a reverse biased Fe/Si Schottky contact and an Fe/AlO3 barrier. For both types of structures the electroluminescence (EL) spectra are dominated by transverse acoustic and optical phonon emissions in the Si. The emitted clear circular polarization of the EL due to radiative recombination in the Si tracks the Fe magnetization, confirming that the spin-polarized electrons originate from the Fe for both types of samples. However, the polarization is lower for the Fe/Si contact than that of the Fe/AlO3/Si system. Systematic TEM analysis has been performed to correlate the interface structure with the observed optical polarization, and reveals some Fe/Si intermixing which is absent in the Fe/AlO3/Si structure. [1] B.T. Jonker et al., Nature Physics 3, 542 (2007). This work was supported by ONR and core NRL programs. 1. Jonker et. al., Nat. Phys. 3, 542 (2007) 2. Applebaum et. al., Nat. 447, 295 (2007)

9:12AM P33.00005 Spin Transport in Silicon1. IAN APPELBAUM, University of Delaware — Silicon has been broadly viewed as the ideal material for spintronics due to its low atomic weight, lattice inversion symmetry, and near lack of nuclear spin, resulting in exceptionally long spin lifetime. Despite this appeal, however, the experimental difficulties of achieving coherent spin transport in silicon were overcome for the first time only recently, by using unique spin-polarized hot-electron injection and detection techniques. [1] Our subsequent observations of very long spin lifetimes and transit lengths [2] have impact on prospects for Spintronics as the basis for a new paradigm of information processing.

References:

1Funded by DARPA/MTO and ONR.

9:48AM P33.00006 All-epitaxial heterostructure for tunneling spins into silicon. MAITRI WARUSAWITHANA, DARRELL SCHLORM, Department of Materials Science and Engineering, Penn State University, XUANGLIN KE, PETER SCHIFFER, Department of Physics, Penn State University. — An all-epitaxial spin-tunnel structure has been constructed using molecular-beam epitaxy (MBE). The structure consists of an epitaxial layer of iron (~100 Å thick) on commensurately strained SrTiO3 (~20 Å thick) on (100) Si. The thin SrTiO3 layer serves simultaneously as a tunnel barrier for spin polarized currents and as a protective layer preventing the reaction between iron and the underlying silicon which would lead to the formation of an undesired iron silicide. While the iron film was grown in ultrahigh vacuum, the growth of the SrTiO3 film on silicon was accomplished using molecular oxygen via a sequence of steps by which the formation of an interfacial amorphous silicon dioxide layer is kinetically suppressed. Magnetic measurements indicate strong magnetic anisotropy with the easy axis lying in the plane of the film and a curie temperature above 400 K. Electrical measurements probing spin injection and detection in microfabricated Fe-SrTiO3-Si-SrTiO3-Fe devices, where the ferromagnetic electrodes have different coercive fields due to size anisotropy, will be discussed.
10:00AM P33.00007 Tunneling Characteristics across Nano-Scale Metal Ferric Junction Lines into Doped Si1, JIANG-QING WANG, KEQIANG WANG, JIRI STEHLIK, Binghamton University — Tunneling properties were studied on nanofabricated metal ferric tunnel structures on phosphorus doped silicon by measuring $I-V$ characteristics and differential conductance versus bias over a wide temperature range between 80 K to 325 K. These properties were found to have very weak temperature dependences up to 250 K. Such temperature independencies in transport properties demonstrated tunneling characteristics from metal ferric nano-lines into Si via AlO$_x$ insulating barrier. Nanoscaled spin-dependent tunneling (STD) lines were patterned on doped Si with the injection contacts having the form of long strips with width and separation of 100 nm and several micron long patterned by e-beam lithography. The measured tunneling coefficient was nearly independent of the bias below 1.0 V, and abruptly increases above the threshold, indentifying such threshold as tunneling barrier height. The thermal transport of the active Si region demonstrated a direct correlation between thermal activation of deep levels (of 0.4 eV) in bulk Si and metal-semiconductor tunneling, revealing feasible mechanisms influencing the interfacial transport.

1Work supported by NSF award no. CTS-022138 and by DOE award no. DEFC52004NA25658

10:12AM P33.00008 Tunnel magnetoresistance of spin tunnel contacts to silicon, R. JANSEN, MESA+ Institute for Nanotechnology, University of Twente, B.C. MIN, R.S. PATEL, S.P. DASH, M.P. DE JONG — For the development of silicon-based spintronic devices, careful design of the contacts between ferromagnet and semiconductor is crucial, as the resistance and potential energy landscape critically affects spin flow across the interface. One approach to engineer spin tunnel contacts to Si uses low work function materials, inserted between the ferromagnet (FM) and the insulator of FM/Al2O3/Si tunnel contacts [1]. Here we present another route to tune the properties of FM/Al2O3/Si contacts by exposure of the Si surface to alkali metal atoms, such as Cs, prior to preparation of the tunnel barrier. This is surprisingly effective in reducing the Schottky barrier height, and will present a series of measurements that elucidate the mechanism. Moreover, we show that the band bending near the contact can be inverted, leading to the formation of a two-dimensional electron gas observable in tunneling spectroscopy, and giving rise to novel tunnel magnetoresistance. [1] B.C. Min et al. Nature Materials 5, 817 (2006).

10:24AM P33.00009 Spin blockade at semiconductor/ferromagnet junctions1, MASSIMILIANO DI VENTRA, YURIY PERSHIN, Department of Physics, University of California, San Diego, La Jolla, California 92093-0319, USA — We study theoretically extraction of spin-polarized electrons at nonmagnetic semiconductor/perfect ferromagnet junctions. The outflow of majority-spin electrons from the semiconductor into the ferromagnet leaves a cloud of minority-spin electrons in the semiconductor region near the junction, forming a local spin-dipole configuration at the semiconductor/ferromagnet interface. This minority-spin cloud can limit the majority-spin current through the junction, creating a pronounced spin blockade at a critical current. We calculate the critical spin-blockade current in both planar and cylindrical geometries and discuss possible experimental tests of our predictions. [1] Yu. V. Pershin and M. Di Ventra, Phys. Rev. B 75, 193301 (2007). [2] Yu. V. Pershin and M. Di Ventra, arXiv:0707.4475.

1This work is partially supported by NSF Grant No. DMR-0133075.

10:36AM P33.00010 Spin injection and transport in graphene layers1, WEIHUA WANG, KEYU PI, WENZHONG BAO, KATHY MCCREARY, WEI HAN, JEANIE C. N. LAU, ROLAND K. KAWAKAMI, Department of Physics and Astronomy, UC Riverside — Graphene is an intriguing material system for spintronics research. Due to its low atomic number and low spin-orbit coupling, graphene is an excellent candidate for spin transport. In our past study, we have demonstrated spin-polarized transport in mesoscopic graphite by two-probe spin-valve devices [1]. Recently, we further investigated this topic and fabricated non-local spin-valve devices consisting of single-layer and few-layer graphene. Ferromagnet (FM) and nonmagnetic electrodes are formed by using electron beam (e-beam) lithography and e-beam evaporation. Thin tunnel barriers consisting of magnesium oxide are inserted between graphene layers and FM electrodes to overcome conductivity mismatch and enhance spin injection efficiency. Atomic force microscopy and Auger spectroscopy are used to characterize their morphology and chemical composition. We performed magneto-transport using the Johnson-Silsbee geometry in a cryogenic environment and observed non-local spin signal up to room temperature. This unambiguously demonstrates the spin injection, transport and detection in graphene materials. [1] W.-H. Wang, et. al., Phys. Rev. B (Rapid Communications), in press.

1Supported by ONR, NSF, and CNID

Wednesday, March 12, 2008 9:00AM - 10:30AM – Session P34 Tutorial for Authors and Referees of Physical Review Morial Convention Center 226

9:00AM P34.00001 Tutorial for Authors and Referees — Editors from Physical Review Letters and Physical Review will provide useful information and tips for our less experienced referees and authors. The information presented will be relevant to anyone who is looking to submit to or review manuscripts for any of the APS journals, or to anyone who would like to add to their knowledge and experience of the authoring and refereeing processes. Topics for discussion will include: (1) how to write good manuscripts and useful referee reports; (2) differences between manuscripts and referee reports for PRL and PR; (3) the roles of authors and referees in the review process; etc. Following a short presentation from the editors, there will be a moderated discussion of these and other topics. Questions from the audience will be most welcome. Refreshments will be served.

Wednesday, March 12, 2008 8:00AM - 10:36AM – Session P35 DMP: Focus Session: Materials for Photovoltaics and Photocatalysis II Morial Convention Center 227

8:00AM P35.00001 Multijunction solar cells for concentrator systems: prospects and challenges, ANDREAS W. BETT, Fraunhofer-Institut fur Solare Energie Systeme — No abstract available.
8:36AM P35.00002 Photovoltaic properties of novel titanium oxide nanotubes. EUGEN PANAITESCU1, CHRISTIAAN RICHTER2, LATIKA MENON3, Northeastern University — Ultrafast synthesis of high aspect ratio titanate nanotubes by anodization in chloride ions containing solutions has been reported and furthermore optimized by our group. We are presenting in this paper the results of relative measurements on photovoltaic properties of the chloride nanotubes samples sensitized with ruthenium dye N3, comparing them with samples obtained by other anodization methods, and with anatase nanopowders. Photoreponse parameters like short circuit current, open circuit voltage, maximum power and overall conversion efficiency have been measured under simulated solar radiation. Preliminary results on absolute measurements on dye sensitized solar cells employing these samples will also be presented.

1Physics Department
2Chemical Engineering Department
3Physics Department

8:48AM P35.00003 Enhanced optical absorption by nanocavities inside titania. WEIQIANG HAN, LIJUN WU, ROBERT KLIB, YIMEI ZHU, Brookhaven National Laboratory — Titania, a wide band gap semiconductor, can generate powerful oxidants and reductants by absorbing photon energies. Titania has been extensively used in photoelectrochemical systems, such as dye-sensitized titania, a wide band gap semiconductor, can generate powerful oxidants and reductants by absorbing photon energies. To improve the photoelectivity of titania, several approaches, including doping and metal loading have been proposed. Nanocavities are isolated entities inside a solid and hence are very different from nanoporous, whose pores (often amorphous and irregular) connect together and open to the surface. Dense polyhedral nanocavities inside single-crystalline anatase titania nanorods were successfully synthesized by simply heating titanate nanorods. The size of the nanocavities is typically about 10 nm. The surfaces of the nanocavity polyhedron are determined to be the crystallographic low-index planes of the titania crystal. We found that these dense nanocavities significantly enhance the optical absorption coefficient of titania in the near-ultraviolet region, thereby providing a new approach to increasing the photoelectivity of the titania nanorods in the applications related to absorbing photons. This work is supported by the U. S. DOE under contract DE-AC02-98CH10886 and Laboratory Directed Research and Development Fund of Brookhaven National Laboratory (to W.H.).

9:00AM P35.00004 Charge Separation in layered Titanate Nanostructures: Effect of Ion Exchange induced Morphology Transformation1, O. DIWALD, A. RISS, H. GROTHE, Vienna University of Technology, Institute of Materials Chemistry. J. BERNARDI, Vienna University of Technology, USTEM, E. KNOEZINGER, Vienna University of Technology, Institute of Materials Chemistry, IMC TU WIEN TEAM — Morphology changes induced by surface chemistry can provide important insights into photoexcitation processes on solids which are critical to photovoltaic and photocatalytic applications. We investigated charge separation processes on Nb2Ti3O7 nanowires and scrolled up H2Ti3O7 nanotubes, two types of morphologies which by means of acid/base treatment can reversibly be transformed into each other. Some of the competitive processes photoexcited states undergo can be tracked by means of electron paramagnetic resonance and photoluminescence spectroscopy. A complementarity between efficient charge separation and radiative recombination of photoexcited states was observed and clearly demonstrates the critical influence of morphology and interlayer composition on the photoelectronic properties of layered oxide nanostructures [2]. [1] Riss et al. Nano Lett. 2007, 7, 433-438. [2] Riss et al. Angew. Chem. Int Ed. 2007, anie.200703817, in press

1Financial support from the Austrian Fonds zur Foerderung der wissenschaftlichen Forschung (P17514N11) is gratefully acknowledged.

9:12AM P35.00005 Bandgap Narrowing of Titanium Dioxides via Non-Compensated n-p Co-Doping for Photocatalysis1, WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, BAOHUA GU, M. PARANS PARANTHAMAN, GYULA ERES, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee — Titanium dioxide (TiO2) is a promising photocatalyst for solar hydrogen production from water, yet its photocatalytic efficiency is limited by its intrinsic wide-bandgap nature. In this talk, we present a conceptually new and intuitive approach, termed non-compensated n-p co-doping, to narrow the bandgap of TiO2. The validity of this approach has been demonstrated using first-principles calculations within density functional theory, showing that extra impurity bands are created in the gap region because of the non-compensated nature of the n-p co-doping, resulting in a narrowed bandgap around 2 eV. Moreover, the electrostatic attraction between the n and p dopants enhances their thermodynamic and kinetic solubility in the host semiconductors. Preliminary experimental results confirming the non-compensated n-p co-doping concept will also be presented, together with its applicability to other wide bandgap semiconductors.

1Supported by the DMSE program and grant number DE-FG02-05ER46209 of USDOE, grant number DMR-0606485 of USNSF, and LDRD program of ORNL.

9:24AM P35.00006 The role of bond switches in light-induced defects in amorphous silicon. LUCAS WAGNER, JEFFREY GROSSMAN, University of California, Berkeley — Amorphous silicon(a-Si) thin-film solar cells are promising materials for solar cells, but they suffer from the Staebler-Wronski effect, in which the efficiency degrades over the course of a few hours of light exposure. While there has been progress in mitigating this effect through sample preparation, there is still no clear microscopic explanation for the degradation. Using first principles density functional theory and highly accurate quantum Monte Carlo techniques, we investigate the simplest reaction in a-Si: a bond switch between two neighboring Si atoms. We find that these reactions can create defect states and can be light activated.

9:36AM P35.00007 Time-domain ab initio studies of photoexcited electron’s dynamics at chromophore-semiconductor interfaces. OLEG PREZHDO, University of Washington — No abstract available.

10:12AM P35.00008 First-principle study of the interfacial rehybridization in organic-inorganic composite photovoltaic devices1, GEORGY SAMSONIDZE, FILIPE J. RIBEIRO, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — Composites of organic conjugated polymers and inorganic nanostructures offer cheap but at present inefficient photovoltaic materials. The efficiency of the photovoltaic device is critically dependent on charge transfer and orbital rehybridization at the donor-acceptor interface. In this work we investigate the P3HT/PCBM interface from density functional theory (DFT) based first-principles calculations. We find a strong rehybridization of the conduction band edge states suggesting an efficient route for exciton dissociation at the interface. Using many-body perturbation theory, we compute the quasiparticle corrections on top of the DFT results. These corrections are critical for accurate predictions and to reach agreement with experiment.

1This work was supported by National Science Foundation Grant No. DMR07-05941 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and NPAI.
10:24AM P35.00009 Pulsed optically detected magnetic resonance of intrinsic a-Si:H at low excitation power. SANG-YUN LEE, THOMAS HERRING, University of Utah, CUNGENG YANG, Department of Medicine, University of Hawaii, HEATHER SEIFEL, CHRISTOPH BOEHME, University of Utah, CRAIG TAYLOR, Colorado School of Mines, JIAN HU, FENG ZHU, MV Systems, Golden, CO, ARUN MADAN — For more than 3 decades, there has been much effort devoted to the investigation of recombination processes in hydrogenated amorphous silicon (a-Si:H). Recently, low-temperature pulsed optically-detected magnetic-resonance (pODMR) studies have shown the presence of a variety of qualitatively different recombination mechanisms that influence the photoluminescence of this material [K. Lips, et. al., JOAM, 7, 13 (2005)]. Here, we present similar experiments with comparatively low light excitation densities (60(10) mW/cm², 514nm, cw Ar⁺ Laser). Qualitatively, our measurements confirm the presence of similar spin dependent recombination channels to those seen at high light excitation densities. However, due to the reduced densities of excess charge carriers, the dynamics of these processes are significantly slower. We attribute this behavior to the decreased transition probabilities at increased charge carrier separations.

Wednesday, March 12, 2008 8:00AM - 10:48AM — Session P36 GIMS: Focus Session: X-ray and Neutron Instrumentation and Science Morial Convention Center 228

8:00AM P36.00001 Advances in Neutron Scattering Instrumentation at Oak Ridge National Laboratory. DOUGLAS ABERNATHY, Oak Ridge National Laboratory — Oak Ridge National Laboratory hosts two world-class neutron sources for condensed matter research. The High Flux Isotope Reactor (HFIR) has recently added a cold source to augment the existing high-intensity thermal beams, and the Spallation Neutron Source (SNS) is the most powerful pulsed spallation neutron source in the world. Investments in neutron scattering instrumentation have come to fruition in a current set of high-performance scattering stations in the user program, covering a wide range of diffraction and spectroscopic techniques. Examples of current scientific results include reflectometry from bio-responsive polymer films and the spectroscopy of slow spin dynamics in frustrated magnetic systems. In 2008 an additional 6 instruments will start user operation or commissioning at the SNS, increasing the breadth and depth of scientific possibilities. Novel techniques and new devices in such areas as sample environment and neutron polarization are also under development.

8:36AM P36.00002 Recent developments on polarized neutron scattering at NIST. WANGCHUN CHEN, NIST, Gaithersburg, Maryland and Indiana University, Bloomington, Indiana, JULIE BORCHERS, ROSS ERWIN, JAMES MCVIER, THOMAS GENTILE, JEFFREY LYNN, NIST, Gaithersburg, Maryland, GORDON JONES, Hamilton College, Clinton, New York — ³He neutron spin filters (NSF) employ nuclear spin-polarized ³He gas, produced by optical pumping, and can be used to polarize or analyze neutron beams because of the strong spin dependence of the absorption cross section for neutrons by ³He. At the NIST center for Neutron Research, the polarized ³He NSF program has been developed to enhance the measurement capability in polarized neutron scattering. This technique has been applied in a number of neutron scattering experiments for user instrumentation and instrumentation development. Here we will discuss applications of the ³He NSF devices in polarized small-angle neutron scattering (SANS), polarized neutron reflectometry (PNR), and polarized triple-axis spectrometry (TAS). For these applications, we employ ³He NSF's as both neutron polarizers and neutron filters that are achieved using the adiabatic fast passage nuclear magnetic resonance technique. We will present the results in each of these applications from magnetic nanoparticles on SANS, patterned magnetic thin films on PNR, and the multiferroelectric system on TAS.

8:48AM P36.00003 Neutron detection in boron carbide/Si heterojunctions as functions of time constants and bias voltage¹. NINA HONG, JOHN MULLINS, S. ADENWALLA, Physics and Astronomy, Univ. of Nebraska-Lincoln — True solid-state neutron detectors have the potential to achieve high efficiencies at low mass, size and power. [1,2] Such detectors made from semiconducting boron carbide (BC) allow for neutron capture and charge collection in the same layer. Here we report neutron detection results from p-n heterojunction diodes of boron carbide on n-type Si. Neutron capture efficiency increases with time constant and reverse bias, from 0.15% at 0 bias and short time constant to 0.46% at 19 V and long time constant. Increasing reverse bias increases the depletion width in the BC layer, leading to a higher proportion of charge capture. The long time constants allow for the detection of charge capture in the BC-scope traces show charge capture times of ~ 30 μs (as compared to < 20 ns in Si). These results indicate that the BC layer is playing an active role in neutron detection, capturing neutrons as well as charge. [1] B. W. Robertson, S. Adenwalla, et al., APL, 80, 3644 (2002). [2] E. Day M. J. Diaz, and S. Adenwalla, J. Phys. D: Appl. Phys. 39, 2020 (2006).

¹ Funded by NASA -NNG05GM89G.

9:00AM P36.00004 The effect of Gd doping on the atomic and electronic structure of HfO₂ thin films. IHOR KETSMAN, ANDREI SOKOLOV, KIRILL BELASHCHENKO, PETER DOWBEN, University Nebraska-Lincoln, YAROSLAV LOSOVYJ, Louisiana State University, JINKE TANG, ZHENJUN WANG, University of Wyoming — HfO₂ is a promising oxide for many applications, including high-k gate dielectric for CMOS devices. In addition, Gd-doped HfO₂ could lead to a dilute magnetic semiconductor and provide an efficient neutron detection medium due to huge neutron absorption cross section of Gd. Gd-doped HfO₂ films deposited on both p-type and n-type silicon by PLD retain monoclinic phase at small doping levels, but can be stabilized in fluorite phase by increased doping [1]. At small doping levels, photoemission measurements indicate the presence of similar spin dependent recombination channels to those seen at high light excitation densities. However, due to the reduced densities of excess charge carriers, the dynamics of these processes are significantly slower. We attribute this behavior to the decreased transition probabilities at increased charge carrier separations.

9:12AM P36.00005 Time-dependent small-angle X-ray and neutron scattering studies of solution-mediated nanoparticulate nucleation, growth and alignment. ANDREW J. ALLEN, VINCENT A. HACKLEY, NIST Ceramics Division, Gaithersburg, MD — A remote-controlled, isothermal, circulating fluid flow cell has been developed for small-angle X-ray and neutron scattering (SAXS and SANS) studies of suspensions with online monitoring of flow rate, temperature or conditions, e.g., pH. Used with the small X-ray beams available at 3rd generation synchrotron sources and the nanometer-to-micrometer scale range accessible in ultrasmall-angle X-ray scattering studies, structural characteristics ranging from 1 nm to several micrometers can be measured, in situ and in real time, as a function of changing physical or chemical conditions. Used with time-resolved pinhole SAXS instruments, rapid reaction precursor phenomena at the nanoscale level can be similarly studied. Used in SANS studies, a neutron-adapted version of the flow cell allows real-time contrast variation techniques to further elucidate the structural evolution. Applications will be discussed for real-time studies of solution-mediated nanocrystalline ceramic oxide formation, and Au nanowire alignment in extensional flow.

9:24AM P36.00006 ABSTRACT WITHDRAWN —
9:36AM P36.00007 Dynamical reconstruction of the valence exciton in LiF

PETER ABBAMONTE, University of Illinois, WEI KU, Brookhaven National Laboratory, TIM GRABER, University of Chicago, JAMES REED, SERBAN SMADICI, University of Illinois, ABHAY SHUKLA, Universite Pierre et Marie Curie, JEAN-PASCAL RUEFF, Synchrotron SOLIEL — We have used inelastic x-ray scattering, coupled with recently developed inversion techniques, to reconstruct the structure and dynamics of the valence exciton in the prototype alkali halide LiF. Our inversions, which yield resolutions $\Delta x = 0.533 \text{Å} \text{and } \Delta t = 20.67 \text{as} (2.067 \times 10^{-17} \text{s})$, reveal that the exciton forms in less than 50 as, oscillates with a period of 283 as, and decays after approximately 5 fs. It contains a pronounced $a/3$ internal periodicity, where $a = 4.027 \text{Å}$ is the crystal lattice parameter, that changes little during the course of its life, indicating that this exciton lies very close to the Frenkel limit. Our results resolve a 70 year old controversy about the valence exciton in alkali halides and, when compared to $ab$ initio calculations, demonstrate a simplified theoretical approach to describing excitons in the spirit of strong binding energy.

1This work is supported by the US Department of Energy, Office of Basic Energy Sciences, DE-FG02-07ER46459.

9:48AM P36.00008 Core-hole propagator and resonant inelastic X-ray scattering: exact results within a Baym-Kadanoff-Keldysh approach

ANDRUI SHVAIKA, TARAS MYSAKOVYCH, Institute for Condensed Matter Physics, 79011 Lviv, Ukraine, JAMES FREERICKS, Department of Physics, Georgetown University, Washington, DC 20057 — We solve for the core-hole propagator and the resonant inelastic X-ray scattering (RIXS) response functions in correlated materials by employing dynamical mean-field theory. We focus our attention on the spinless Falicov-Kimball model, where the problem can be solved exactly, and the system can be tuned to go through a Mott-Hubbard-like metal-insulator transition (the coupling with the core hole is also a Falicov-Kimball type of interaction). The core-hole propagator is expressed in terms of a continuous fermionic Toepplitz determinant defined only on the upper real-time branch of the Keldysh contour. We have derived exact large-time asymptotics for the core-hole propagator using the Wiener-Hopf finite sum equation technique which produces an efficient algorithm to obtain the density of states of the X-ray edge problem for any temperature and any interaction strength. We have also derived the two-particle vertices in a diagrammatic representation of the scattering processes (using a Baym-Kadanoff-Keldysh approach). As an example of this formalism, we show results for the L-edge contributions to RIXS. This work was supported by Award No. UKP2-2697-LV-06 of the U.S. Civilian Research and Development Foundation.

10:00AM P36.00009 Identification of Mn site in Pb(Zr,Ti)O$_3$

A. BOONCHUN, M. F. SMITH, S. RUJIRAWAT, B. CHERDHIRUNKORN, S. LIMPIJUMNONG, School of Physics, Suranaree University of Technology, Thailand — The impurity Mn in PbTiO$_3$ and PbZrO$_3$ has been studied by means of first-principles spin density functional theory. It is found that the Mn atom energetically prefers to substitute on the Ti/Zr site over other sites (i.e., Pb site, O site or interstitial) under all equilibrium growth conditions. The calculations predict that a majority of Mn atoms substitute for Ti/Zr and have neutral-charge state each with a total electron spin of $M = 3/2$. This prediction is supported by the combination of x-ray absorption near edge structure (XANES) experiment and first-principles simulation of the spectrum. The measured XANES of the Mn-doped Pb(Ti,Zr)O$_3$ within the concentration range of 0.5 - 2.0 at% yield the exact same features, indicating that the location of Mn in the crystal is independent of Mn concentration. The measured XANES is consistent with the partial density of states simulation of Mn atom on the Ti/Zr site and inconsistent with the simulations of Mn atom on other sites.


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10:12AM P36.00010 Direct mapping of phonon dispersions in copper by x-ray thermal diffuse scattering

RUQING XU, HAWOONG HONG, TAI CHIANG, University of Illinois at Urbana-Champaign — X-ray Thermal Diffuse Scattering (TDS) arises from lattice vibrations. Measured TDS intensities can be used to extract phonon dispersion relations, as has been demonstrated in a number of systems. But most analysis methods so far have involved data fitting based on assumed atomic force constant models, and it is difficult to determine a priori the accuracy of the procedure. Methods of direct inversion, i.e., deterring k-space frequencies directly from x-ray TDS data without a presumed model, have been proposed in prior work, but most of the schemes involve absolute intensity measurements, which are difficult especially in the presence of an unknown background. Here we report an improved approach, in which phonon frequencies are determined through the temperature dependence of TDS intensities at each point in reciprocal space. Polarization selection rules are employed to disentangle contributions from different phonon branches. Results taken from a simple model material, copper, will be presented.

10:24AM P36.00011 Fractionation of uranium isotopes in minerals screened by gamma spectrometry

JEFFREY L. GEIGER, AUSTIN M. BALDWIN, CHARLES C. BLATCHLEY, Pittsburg State University — At least two groups have reported finding shifts in the ratio U-235/U-238 for sandstone, black shale, and other sedimentary samples using precision ICP-MS. These shifts were tentatively attributed to a recently predicted isotope effect based on nuclear volume that causes fractionation for U-235/238. However, fractionation of high Z elements may be less likely an explanation than U-235 depletion induced by galactic cosmic ray neutrons. Isotope depletion in marine sediments could therefore be an indicator of changes in cosmic ray flux due to nearby supernovae, gamma-ray bursts, or longer term changes during the 62 million year cycle of high Z elements. We report using a less precise approach than ICP-MS, but one which can quickly screen samples to look for anomalies in isotope ratios, namely HPGe gamma ray spectrometry. Various levels of depletion were measured for uranium rich minerals, including brannerite, carnottite, and pitchblende, as well as coal and limestone samples.

1Partially funded by NASA EPSCoR 2006 and KTEC.

10:36AM P36.00012 Electronic Structure Study of Cerium Doped Scintillators

DA GAO, MICHAEL MCLIVAIN, Idaho National Laboratory — The interest shown in recent years related to cerium doped lanthanide halides, such as LaCl$_3$, LaBr$_3$, and LaI$_3$, is mainly due to their potential applicability as gamma ray scintillation detectors. We have performed a comprehensive theoretical study of these materials to better understand the scintillation process and define the nature of the self trapped exciton (STE) associated with thermally dependent scintillation process. The present work focuses on the study of the luminescence properties of cerium doped lanthanide halide scintillators from the point of view of solid state band structure calculations. Our calculated band structures are in good agreement with experimental values. For example, LaCl$_3$ band gap is calculated to be 6.85 eV as compared to approximately 7.0 eV for the experimentally determined value. The theoretically calculated excitation spectra are also compared with the experimental spectra. We find that scintillation efficiency is dependent on the location of the of Ce$^{3+}$ ground 4f and excited 5d levels with respect to the fundamental band gap of the host materials.

1This work was supported by the U.S. Department of Energy, Office of Biological and Environmental Research, Environmental Research Science Program under Contract No. DE AC07-05ID14517.
We report photoluminescence (PL) measurements of GaAs incorporation is predicted to mainly perturb the valence band and does not significantly affect the electron mobility, thus promising better device performance. Bi\textsubscript{GaAs} with small amounts of N or Bi results in a large reduction of the fundamental band gap, leading to the so called “giant band gap bowing”. GaAs doping with magnetic versus non-magnetic impurities. Effects of disorder, compensation, and doping in these samples. In addition, comparing Mn doped and Be doped films allows for distinguishing the effects of doping and compensation.

The work was supported by the Semiconductor Research Corporation. NCN computational resources were used.

3Supported by the NIH, the NSF, and the WU CMI

8:36AM P37.00004 Micro-spectroscopy of Ga\textsubscript{1−x}Mn\textsubscript{x}As and Ga\textsubscript{1−x}Be\textsubscript{x}As films with gradient doping and compensation, BRIAN CHAPLER, University of California San Diego, R.C. MYERS, D.D. AWSCHALOM, University of California Santa Barbara, M.C. MARTIN, Lawrence Berkeley National Laboratory, K.S. BÜRCH, Los Alamos National Laboratory, D.N. BASOV, University of California San Diego — A detailed study into the problem of carrier induced magnetism in ferromagnetic III-Mn-V semiconductors is being carried out using micro-infrared measurement techniques. Infrared micro-spectroscopy and broad-band micro-ellipsometry measurements have been performed on films of Ga\textsubscript{1−x}Mn\textsubscript{x}As, \( x = 0.03, 0.16\), as well as Ga\textsubscript{1−x}Be\textsubscript{x}As, \( x = 0.018\). The films were prepared using non-rotated molecular beam epitaxial growth. The results of this growth are films with a varying As:Ga ratio across the sample. Using the above experimental techniques, measurements can be taken at specific locations along the As:Ga gradient, which have shown to cause systematic changes in spectra as a function of As:Ga ratio. These experiments provide a unique opportunity to study the effects of disorder, compensation, and doping in these samples. In addition, comparing Mn doped and Be doped films allows for distinguishing the effects of doping with magnetic versus non-magnetic impurities.

8:48AM P37.00005 Slow light and anomalous pulse breakup near an exciton resonance in GaAs quantum wells, TIMOTHY SWEENEY, YAN GUO, SUSANTA SARKAR, HAILIN WANG, Department of Physics, University of Oregon, Eugene, OR 97403 — We report experimental studies of optical pulse propagation near an exciton resonance in GaAs quantum wells. The spectral dependence of the group velocity reveals a sharp decrease in the group delay when the spectral position of the optical pulse is varied from below to above the exciton absorption line center. The decrease in the group delay occurs in a spectral range that is small compared with the exciton absorption linewidth. Pulse breakups are also observed when input optical pulses with relatively low intensities are slightly below the exciton absorption line center. Detailed nonlinear optical studies suggest that these surprising behaviors arise from coherent population oscillation and especially a sharp increase of the exciton decoherence rate from below to above the exciton absorption line center.

9:00AM P37.00006 ABSTRACT WITHDRAWN —
9:24AM P37.00008 Effect of spin-orbit coupling on excitonic levels in layered chalcogenide-
fluorides, ANDRIY ZAKUTAYEV, ROBERT KYKYNESHI, JOSEPH KINNEY, DAVID H. MCINTYRE, GUENTER SCHNEIDER, JANET TATE, Department of Physics, Oregon State University — BaCuCHF (Ch=S,Se,Te) comprise a family of wide-bandgap p-type semiconductors. Due to their high transparency and conductivity, they have potential applications as components of transparent thin-film transistors, solar cells and light-emitting devices. Thin films of BaCuCHF have been deposited on MgO by pulsed laser deposition (PLD). Solid solutions BaCuSi$_1-x$Se$_x$Te$_x$ and BaCuSe$_1-x$Te$_x$ have been prepared by PLD of alternating thin BaCuCHF layers. All films were deposited at elevated substrate temperatures. They are preferentially c-axis oriented, conductive and transparent in the visible part of the spectrum. Double excitonic peaks have been observed in the absorption spectrum of these films in the temperature range from 80 to 300K. The separation between the peaks in the doublet increases with the increase of atomic mass of the chalcogen. It also increases with the increase of the heavy chalcogen component $x$ in the solid solutions. This separation most likely is caused by the effect of spin-orbit coupling in the chalcogen atoms on excitonic levels in BaCuCHF.

9:36AM P37.00009 Photocurrent-induced transport of exciton energy in a single heterojunction quantum well, PATRICK FOLKES, Army Research Laboratory, YINGMEI LIU, University of Pittsburgh — Excitons which coexist with a degenerate two-dimensional electron gas (2DEG) in the same quantum well subband have been observed in the photoluminescence (PL) from the recombination of electrons with localized photoexcited holes. Under pulsed photoexcitation at a critical applied voltage, the screening response of the 2DEG/exciton system to the appearance of a remote photocurrent filament in the 2DEG results in the existence of spatially direct and red-shifted indirect excitons in the photoexcitation region and the anomalously fast formation of in-plane spatially indirect excitons which are localized around the filament. Our data suggests the occurrence of a fast long range transport of exciton energy.

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9:48AM P37.00010 Two-dimensional hole systems in InSb and In$_x$Ga$_{1-x}$As quantum wells, CHOMANI GASPE, MADHAVIE EDIRISOORIYI, TETSUYA MISHIMA, MICHAEL SANTOS, University of Oklahoma — CMOS circuits require $p$-type transistors with high hole mobility, in addition to $n$-type transistors with high electron mobility. In InSb, we have observed room-temperature electron mobilities of 10,000 and 40,000 cm$^2$/Vs in quantum wells made of In$_{0.5}$Ga$_{0.47}$As and InSb, respectively. To achieve high hole mobilities, strain and confinement must be maximized. Both parameters increase the energy splitting between holes with light in-plane mass and those with heavy in-plane mass. We have observed a room-temperature hole mobility of 600 cm$^2$/Vs in InSb quantum wells with remotely Be-doped Al$_x$In$_{1-x}$Sb barriers grown on GaAs substrates by molecular beam epitaxy. We will discuss the effects of strain, structural parameters, and defect density on hole mobility in InSb and In$_x$Ga$_{1-x}$As quantum wells.

10:00AM P37.00011 ABSTRACT WITHDRAWN —

10:12AM P37.00012 Non-Markovian damping of Rabi oscillations in semiconductor quantum dots, LUIZ E. OLIVEIRA, Instituto de Física - Unicamp - Brazil, DMITRI MOGILEVTSEV, A.P. NISOVTSEV, S. KILIN, Instituto de Física - NASB - Belarus, S.B. CAVALCANTI, Instituto de Física - UFAL - Brazil, H.S. BRANDI, Instituto de Física - UFRJ - Brazil — A systematic investigation is performed on the damping of Rabi oscillations induced by an external electromagnetic field interacting with a two-level semiconductor system. We have considered a coherently driven two-level system coupled to a dephasing reservoir, and shown that in order to explain the dependence of the dephasing rate on the driving intensity, it is essential to consider the non-Markovian character of the reservoir. Moreover, we have demonstrated that intensity-dependent damping may be induced by various dephasing mechanisms due to stationary as well non-stationary effects caused by the coupling with the environment. Finally, present results [1] are able to explain a variety of experimental measurements [2-4] available in the literature.


10:24AM P37.00013 Nonlinear Terahertz pump-Terahertz probe Measurements of Semiconductor Carrier Dynamics, HAIDAN WEN, AARON LINDENBERG, PULSE Center, Stanford Linear Accelerator Center, LINDENBERG LAB TEAM — A table-top terahertz (THz) source has been employed to study the nonlinear response of semiconductors to near-half-cycle femtosecond pulses in the THz regime. We report nonlinear field-induced changes in the far infrared absorption coefficient induced by THz pulses. The transmittance as the function of THz peak field was measured using a z-scan technique and it is observed that the absorption coefficient dramatically increases above a threshold field.

1Department of Materials Science and Engineering, Stanford University

10:36AM P37.00014 Effect of Spin-Orbit Interaction on the Lattice Properties of Solids: Sb and Bi, M. CARDONA, MPI fuer Festkörperforschung, D-70569 Stuttgart, Germany, L. E. DIAZ-SANCHEZ, CINESTAV-Queretaro, 76230 Queretaro, Qro., Mexico, X. GONZE, Unite de Physico-Chimie et de Physique des Matériaux, Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium, R. K. KREMER, MPI fuer Festkörperforschung, D-70569 Stuttgart, Germany, A. H. ROMERO, CINESTAV-Queretaro, 76230 Queretaro, Qro., Mexico, J. SERRANO, ICREA, EPSC Universitat Politècnica de Catalunya, 08860 Castelldefels, Spain — We present measurements of the specific heat ($C$) vs. $T$ for Bi and Sb and vs. isotopic mass for Sb. The measurements are compared with $ab$-initio calculations performed with the ABINIT code, including spin-orbit (S-O) interaction. It is shown that the S-O interaction softens the lattice and thus increases the value of $C$ at the low $T$ maximum ($T_m \sim$8K for Bi, $T_m \sim$14K for Sb), improving agreement between theory and experiment. The effect of S-O interaction on other thermodynamic properties, such as the lattice parameter, $a_0$, and the cohesive energy, $E_c$, is also calculated. It is shown that this interaction decreases $E_c$ and, correspondingly, increases $a_0$. These effects are proportional to $c_2 \lambda^2 + c_3 \lambda^4$, where $\lambda$ is the S-O coupling constant, about twice as large for Bi as for Sb.

Wednesday, March 12, 2008 8:00AM - 11:00AM –
Session P38 DCMP: Relaxor Ferroelectrics and Piezoelectrics Morial Convention Center 230
We have discovered that by substituting the 'A' site with a smaller atom compared to Pb to apply “chemical pressure” and tune the morphotropic-phase boundary to lower pressures.

Laboratory, HAOSU LUO, Shanghai Institute of Ceramics — The lattice dynamics of PbMg1/3Nb2/3O3extremely high piezoelectric coefficient, higher electromechanical coupling, and larger attainable bandwidth. This will lead to enhanced agility of NEMS/MEMS devices. The main advantages are the materials are extremely important for applications in micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS). Here, we will be presenting PMN-PT (Lead Magnesium Niobate-Lead Titanate) on SOI as a hyper piezoelectric material for NEMS devices. The main advantages are the materials are extremely important for applications in micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS). Here, we will be presenting PMN-PT (Lead Magnesium Niobate-Lead Titanate) on SOI as a hyper piezoelectric material for NEMS devices.

Material Science and Engineering, Pennsylvania State University, PA 16802, VLADIMIR AKSYUK, Alcatel-Lucent Technologies, NJ 07974 — Piezoelectric BLICK, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706, SEUNG-HYUB BAEK, CHANG-BEOM EOM, MUHTAR AHART, RONALD E. COHEN, RUSSELL J. HEMLEY, Carnegie Institution of Washington — Motivated to determine and understand PMN-32%PT’s behavior under pressure, we employed the angular dispersive x-ray diffraction methods (Advanced Photon Source, Argonne National Laboratory) to investigate PMN-32%PT in a diamond anvil cell up to 15 GPa. The x-ray diffraction results show changes in Bragg peaks at 4 GPa which indicate that PMN-32%PT undergoes a ferroelectric rhombohedral to a paraelectric cubic phase transition. In addition, we investigated the pressure dependence of domain structure of PMN-32%PT up to 10 GPa; rhombohedral domains decrease with pressure and disappear above 4 GPa. These results are qualitatively consistent with earlier Raman study of B. Chaubane, (Phys. Rev. B 70, 134114, 2004). We suggest a phase diagram for PMN-PT system which is slightly different from the one predicted by B. Chaubane et al.

1This work is supported by the ONR under the contract number N000140215056 and the Carnegie/Department of Energy Alliance Center (CDAC) (DF-FC030000144).

8:36AM P38.00004 Aging mechanisms in field cooled PMN-PT 12%, MATTHEW DELGADO, EUGENE COLLA, MICHAEL WEISSMAN, University of Illinois Urbana-Champaign — In the relaxor ferroelectric PMN-PT 12% ((PbMg1/3Nb2/3O3)0.98(PbTiO3)0.02) the dielectric susceptibility (ε″, ε′′) and pyroelectric current I₀ were measured after different field-temperature histories. As previously reported [1], when the sample was cooled in zero field, standard spinglass-like aging of ε″ was found in the glassy relaxor regime. Cooling in a DC electric field of 0.67 kV/cm drove a transition into a polarized ferroelectric-like state, which retained its polarization after the field was removed at low temperature. During 10 hours of subsequent zero-field aging at 160K, ε″ showed almost no change. This suggests that the mechanisms responsible for glasisy aging in the relaxor state are absent in the ferroelectric state. [1] L. Chao, et al. PRB 74, 014105 (2006).

8:48AM P38.00005 Hyper Piezoelectric Nano-Electromechanical Systems, DUSTIN KREFT, ROBERT BLICK, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706, SEUNG-HYUB BAEK, CHANG-BEOM EOM, Department of Material Science and Engineering, University of Wisconsin-Madison, WI 53706, V. VAITYHANATHAN, DARRELL SCHLOM, Department of Material Science and Engineering, Pennsylvania State University, PA 16802, VLADIMIR AKSYUK, Alcatel-Lucent Technologies, NJ 07974 — Piezoelectric materials are extremely important for applications in micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS). Here, we will be presenting PMN-PT (Lead Magnesium Niobate-Lead Titanate) on SOI as a hyper piezoelectric material for NEMS devices. The main advantages are the extremely high piezoelectric coefficient, higher electromechanical coupling, and larger attainable bandwidth. This will lead to enhanced agility of NEMS/MEMS devices and lower energy consumption. The work will also have considerable impact for nanoscale mechanics.

9:00AM P38.00006 Zone Boundary Soft Modes in Relaxor PMN, PETER GEHRING, NIST Center for Neutron Research, JAN SWAINSON, NRC, Chalk River Laboratories, CHRIS STOCK, ISIS, Rutherford Appleton Laboratory, GUANGYONG XU, Brookhaven National Laboratory, HAOSU LUO, Shanghai Institute of Ceramics — The lattice dynamics of PbMg1/3Nb2/3O3, a prototypical relaxor, have been studied using neutron TOF techniques at the NIST Center for Neutron Research. Unusual “columns” of inelastic scattering are seen at the M and R-point zone boundaries of 300K. These columns are due to the superlattice peaks observed in the relaxor regime. Preliminary neutron structure factor calculations indicate that the corresponding ionic displacements involve the Mg/Nb and Pb atoms. This picture is consistent with x-ray studies according to which the superlattice peaks result from <110> correlated, anti-parallel Pb displacements. The potential relationship between the columns and superlattice peaks is intriguing because the temperature dependence of the M-point superlattice peak tracks that of the soft, zone center mode, which is associated with the development of short-range ferroelectric correlations. [1] A. Tkachuk and H. Chen, AIP Conf. Proc., 677, p. 55 (2003); [2] P. M. Gehring, S. Wakimoto, Z.-G. Ye, and G. Shirane, Phys. Rev. Lett. 87, 277601 (2001).

9:12AM P38.00007 Polar nanoregions and phase instability in relaxors, GUANGYONG XU, Brookhaven National Laboratory, JINSHENG WEN, Brookhaven National Lab/Stonybrook, CHRISTOPHER STOCK, Rutherford Appleton Lab, U.K., PETER GEHRING, NIST — Local polar clusters called polar nano-regions (PNR) are believed to play important roles in the electronic properties of relaxor ferroelectrics. Recent work has shown that the presence of PNRs in relaxor systems could also be related to the high piezoelectric response in these materials. Diffuse scattering studies on PNRs in PMN-xPT and PZN-xPT systems will be presented and their electric field response will be discussed. Our results suggest that there is an intrinsic phase instability in relaxor systems induced by the PNRs, which makes it easier for an (electric field) induced strain to develop. Possible scenarios for the further enhancement of the piezoelectric response near the morphotropic phase boundary (MPB) will also be discussed.
9:24AM P38.00008 First-Principles Investigations of Pb Anti-Site Defects in PbZrO$_3$ and Pb(Zr, Ti)O$_3$ Perovskites$^1$. RICARDO KAGIMURA, DAVID J. SINGH, Oak Ridge National Laboratory — Lead zirconate (PZ) and lead zirconate titanate (PZT) have the perovskite type structure, ABO$_3$. Bivalent lead (Pb$^{2+}$) ions occupy the A site, while tetravalent titanium and zirconium (Zr$^{4+}$, Ti$^{4+}$) ions occupy the B site at random of the PZT solid solution. Also, lead can be tetravalent (Pb$^{4+}$), such as in PbO$_2$ structure. Recent experimental work has reported that tetravalent Pb ions can locate at the B site of the PZT perovskite forming a lead zirconate-titanate-plumbate solid solution. The experimental results suggest that, based on a PbZrO$_3$-PbTiO$_3$-PbPbO$_{3}$ ternary solution phase diagram [G. Suchaneck et al., Ferroelectrics 318, 3 (2005)], the substitutional Pb atom prefers to occupy the Zr site instead of the Ti one. In this work, we report density functional supercell calculations for pure PbZrO$_3$ perovskite and for ordered Pb(Zr$_{1/2}$Ti$_{1/2}$)$_3$O$_9$ solid solution with different configurations for the Zr and Ti atoms. We investigate the anti-site defect energies and the effects on the electronic structure.

$^1$This work was supported by the Department of Energy ORNL LDRD program and Division of Materials Science and Engineering, and by the Office of Naval Research. One of the authors (R. K.) also was supported by the Brazilian agency - CNPq.

9:36AM P38.00009 Stability of point defects in SrTiO$_3$ substrates during thin film deposition. EMMANUEL TOWEY, SHEHNAZ JEDDY, GREGG JANOWSKI, Abant Izzet Baysal University, Department of Physics — We will report the results of a first principles investigation of the electronic and lattice dynamical properties of so-called giant dielectric compound Na$_{1/2}$Bi$_{1/2}$Cu$_3$Ti$_4$O$_{12}$ which was found to have a very high ‘extrinsic’ as well as ‘intrinsic’ dielectric constant. The calculations have been carried out within the local spin density functional approximation using norm-conserving pseudopotentials and a plane-wave basis. The electronic band structure suggests that, based on a PbZrO$_3$-PbTiO$_3$-PbPbO$_{3}$ ternary solution phase diagram [G. Suchaneck et al., Ferroelectrics 318, 3 (2005)], the substitutional Pb atom prefers to occupy the Zr site instead of the Ti one.

9:48AM P38.00100 Electron Beam Excitation Mechanism of Rare Earth Ions in LiNbO$_3$. T. TAFOIN PENN, V. DIEROLF, G.S. CARGILL III, Lehigh University — Many applications of ferroelectric materials in frequency conversion are based on precise engineering of the ferroelectric domains. Unfortunately, the quest for smaller feature sizes is slowed due to the lack of real-time local controls of the process. We explored the feasibility of using as local probes RE ions in LiNbO$_3$ that exhibit in their excitation and emission spectra linear Stark shifts making them sensitive to local electric fields such as local charging and fields from defect dipoles. We studied the feasibility of this approach for the domain writing process induced by an e-beam in a SEM. A necessary first step is a good understanding of the excitation mechanisms of RE:LiNbO$_3$ that leads to CL under e-beam irradiation. We observe a pronounced saturation already for moderate e-beam currents indicating that not all RE ions can be excited. This excludes the direct excitation pathway as a major contributor to the CL excitation. Our observations are explained by a defect trap mediated energy transfer between generated electron-hole pairs and the RE ions. Independent of the RE ion, we find that the energy transfer rate from the defect trap to the RE ion is less than 100 ns$^{-1}$.

1Supported by ARO-Grant W911NF-04-1-0032.

10:00AM P38.00011 Raman study of the phonon modes in bismuth pyrochlores$^1$. DANIEL ARENAS, WEI QIU, JUAN NINO, DAVID TANNER, University of Florida, LEV GASPAROV, University of North Florida — The Raman Spectra of the cubic bismuth pyrochlores Bi$_2$Zn$_2$Nb$_2$O$_9$, Bi$_3$ZnTa$_3$O$_{12}$, Bi$_2$MgNb$_2$O$_{12}$, and Bi$_3$MgTa$_3$O$_{12}$ were measured. The samples, in ceramic form, were measured from 50 to 1000 cm$^{-1}$ at room temperature. The Raman bands were tentatively assigned to specific vibrational modes. Overall, the Raman spectra were similar for all four samples and the number of modes was affected by the displacement disorder in the bismuth-based compounds. The results will also be compared to published infrared data to gain insight into these additional modes. Last, the existence of an 860 cm$^{-1}$ mode in BiZn and BMNb will be discussed as it suggests influence of the lone pair character on the displacement disorder.

$^1$Supported by the DOE through DE-FG02-02ER45984 and by the NHMFL.

10:12AM P38.00012 A Low-Temperature Specific Heat Study of the Giant Dielectric Constant Materials. C. P. SUN, J. Y. LIN, H. D. YANG, Department of Physics, National Sun Yat-Sen University, Kaoshuing 804, Taiwan, Republic of China, JIANJUN LIU, CHUN-GANG DUAN, W. N. MEI, Department of Physics, University of Nebraska at Omaha, Nebraska, 68182-0266, USA — Low-temperature specific-heat study has been performed on the insulating giant dielectric constant material CaCu$_3$Ti$_4$O$_{12}$ and two related compounds, Bi$_2$Cu$_3$Ti$_4$O$_{12}$ and La$_2$Na$_{0.5}$Cu$_3$Ti$_4$O$_{12}$, from 0.6 to 10 K. From analyzing the specific heat data at very low-temperature range, 0.6 to 1.5 K, and moderately low-temperature range, 1.5 to 5 K, in addition to the expected Debye terms, we noticed significant contributions originated from the linear and Einstein terms, which we attributed as the manifestation of low-lying elementary excitations due to lattice vibrations occurred at the grain boundaries and induced by local defects. Together with the findings on electronic and mechanical properties, a phenomenological model is proposed to explain the high dielectric constant behaviors at both low and high frequency regions.

10:24AM P38.00013 First Principles Investigation of Electronic and Lattice Dynamical Properties of High Dielectric Constant Material Na$_{1/2}$Bi$_{1/2}$Cu$_3$Ti$_4$O$_{12}$. CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Department of Physics — We will report the results of a first principles investigation of the electronic and lattice dynamical properties of so-called giant dielectric compound Na$_{1/2}$Bi$_{1/2}$Cu$_3$Ti$_4$O$_{12}$ which was found to have a very high ‘extrinsic’ as well as ‘intrinsic’ dielectric constant. The calculations have been carried out within the local spin density functional approximation using norm-conserving pseudopotentials and a plane-wave basis. The ground state is found to be antiferromagnetic direct-band gap semiconductor. Lattice dynamical properties, such as Born effective charge tensors, dielectric permittivity tensors, and phonon frequencies at the Brillouin zone center were calculated using density functional perturbation theory and found to be similar to more studied CaCu$_3$Ti$_4$O$_{12}$ and CaCu$_3$Ti$_4$O$_{12}$ compounds. The calculated electronic ($\epsilon_{\text{el}} \approx 11.5$) and static ($\epsilon_{\text{st}} \approx 150$) dielectric constants indicate that the observed high dielectric constant is extrinsic in origin. The main contribution to the static dielectric constant is found to be due to a low frequency (50 cm$^{-1}$) IR-active mode which has a large mode effective charge.

$^1$This work was supported by TUBITAK under grant no. TBAG-2449(104T057) and AIBU Research Fund grant no. 04.03.02.199
Transition temperature of martensitic transformations in hafnia and zirconia

XUHUI LUO, UT Austin, A.A. DEMKOV, UT Austin — Transition metal oxides find applications in ceramics, catalysis and semiconductor technology. In particular, hafnium dioxide or hafnia will succeed silica as a gate dielectric in advanced transistors. However, thermodynamic properties of thin hafnia films are not well understood, despite their technological importance. We use density functional theory to investigate the tetragonal to monoclinic phase transition in hafnia and zirconia. We find that unlike the case of the cubic to tetragonal transition, this phase transition is not driven by a soft mode. We use transition state theory to identify the minimum energy path (MEP) employing first principle calculations for hafnia and zirconia, sow that both transformations are martensitic, and obtain the transition barriers. Martensitic transformations include both the internal coordinate transformation and deformation of the cell lattice vectors ("strain and shuffle”), therefore the potential energy surface and MEP are function not only of the internal atomic coordinates but also of the unit cell lattice vectors. Considering the simplest case of uniform strain the transition temperatures we then relate the barrier height to the transition temperature. As a self-consistency check, assuming the equality of thermodynamics potentials of the tetragonal and monoclinic phases during the transition, and using the difference in the internal energy calculated from first principles we estimate the entropy change associated with the transition which is found in good agreement with that calculated form the phonon spectra.

Correlation effects in charge-density wave insulator BaBiO3

CESARE FRANCHINI, MARTIJN MARSMAN, GEORG KRESSE, Faculty of Physics, University of Vienna and Center for Computational Materials Science — The negative-U nature of BaBiO3 leads to a charge-ordered insulating state in which pentavalent Bi5+ coexists with trivalent Bi3+. Despite the apparent absence of strong-correlation effects in BaBiO3 standard density functional (DFT) theory yields a much too small band gap of 0.14 eV. By means of an hybrid-DFT approach combined with self-consistent GW including vertex corrections we investigate the electronic, vibrational and dielectric properties of BaBiO3. We show that the inclusion of strong-correlation effects increases the band gap up to 1.2 eV, shifts the oxygen breathing modes upwards by ≈ 2 THz and reduces the dielectric constant by a factor of 3. The overall agreement with available experimental data is significantly improved.

Effects of quenched randomness on predator-prey interactions in a stochastic Lotka-Volterra lattice model

UWE C. TAUBER, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435, ULRICH DOBRAMYSL, Institute of Semiconductor and Solid State Physics, Johannes Kepler University, 4040 Linz, Austria — We study the influence of spatially varying reaction rates (i.e., quenched randomness) on a stochastic two-species Lotka-Volterra lattice model for predator-prey interactions using Monte Carlo simulations. The effects on the asymptotic population densities, transient oscillations, spatial distributions, and on traveling wave and invasion front speed are investigated. We find that spatial variability in the predation rate yields an increase in the asymptotic population densities of both predators and prey.

Effects of quenched randomness on predator-prey interactions in a stochastic Lotka-Volterra lattice model

PER ARNE RIKVOLD, VOLKAN SEVIM, Florida State University — We report very long kinetic Monte Carlo simulations of eco- systems generated by individual-based models of biological co-evolution, emphasizing the temporal fluctuations in community structure, diversity, and population sizes [1-3]. These multispecies coevolution models contain both producers that directly utilize an external resource, and consumers that must consume one or more other species for support. Time series of diversities and population sizes over tens of millions of generations display highly correlated fluctuations that give rise to power spectra of 1/f form. These model-intrinsic dynamic features correspond to large, correlated extinction events and similarly correlated bursts of new species, without the need for external catastrophic events. The communities generated by the evolution process take the form of simple food webs, whose species abundance distributions and degree distributions are consistent with data from real food webs.

Research in part funded through the National Science Foundation, NSF DMR-00755725, and supported through an IAESTE student exchange internship.

Dynamical Clustering in Reaction-Dispersal Processes on Complex Networks

VINCENT DAVID, MPI-DS, Gottingen, MARC TIMME, MPI-DS, BCCN, Gottingen, THEO GEISEL, University of Gottingen, MPI-DS, BCCN, Gottingen, DIRK BROCKMANN, Northwestern University, Evanston — We investigate nonlinear annihilation processes (e.g., A + A → 0) of particles that perform random walks on complex networks. In well mixed populations (mean field) this process exhibits t−1 decay behavior in the total number of particles. Additional dispersal of particles adds a second time scale and drastically changes the decay behavior. Here we study these changes for two types of hopping processes. First, if particles independently select one of the possible exit channels at each node their exit rates are given by the sum of all outgoing weights such that the waiting times are degree-dependent. We compare this to the popular ansatz of a uniform waiting time process. Derived mean field equations show that for large numbers of particles per node both processes exhibit nearly identical relaxation properties. However, below a critical particle number the processes deviate not only from mean field predictions but, more importantly, by orders of magnitude from one another. We attribute this to dynamical clustering effects in the uniform waiting time model, that is absent in the independent channel dynamics.

Fluctuations and Food-web Structures in Individual-based Models of Biological Coevolution

PER ARNE RIKVOLD, VOLKAN SEVIM, Florida State University — We report very long kinetic Monte Carlo simulations of eco- systems generated by individual-based models of biological co-evolution, emphasizing the temporal fluctuations in community structure, diversity, and population sizes [1-3]. These multispecies coevolution models contain both producers that directly utilize an external resource, and consumers that must consume one or more other species for support. Time series of diversities and population sizes over tens of millions of generations display highly correlated fluctuations that give rise to power spectra of 1/f form. These model-intrinsic dynamic features correspond to large, correlated extinction events and similarly correlated bursts of new species, without the need for external catastrophic events. The communities generated by the evolution process take the form of simple food webs, whose species abundance distributions and degree distributions are consistent with data from real food webs.

Support from NSF-DMR 0240078 and NSF-DMR-0444051 acknowledged.

Metabolic disease network and its implication for disease comorbidity

DEOK-SUN LEE, Northeastern University, ZOLTAN OLTVAI, University of Pittsburgh, NICHOLAS CHRISTAKIS, Harvard Medical School, ALBERT-LASZLO BARADASI, Northeastern University — Given that most diseases are the result of the breakdown of some cellular processes, a key aim of modern medicine is to establish the relationship between disease phenotypes and the various disruptions in the underlying cellular networks. Here we show that the current understanding of the structure of the human metabolic network can provide insight into potential relationships among often distinct disease phenotypes. Using the known enzyme-disease associations, we construct a human metabolic disease network in which nodes are diseases and two diseases are linked if the enzymes associated with them catalyze adjacent metabolic reactions. We find that the more connected a disease is, the higher is its prevalence and the chance that it is associated with a high mortality. The results indicate that the cellular network-level relationships between metabolic pathways and the associated disease provide insights into disease comorbidity, with potential important consequences on disease diagnosis and prevention.
8:48AM P39.00005 The Human Phenotypic Disease Network, CESAR HIDALGO, Center for Complex Network Research, Dept of Physics, University of Notre Dame, NICHOLAS BLUMM, Center for Network Science, Dept of Computer Science, Northeastern University, ALBERT-LASZLO BARABASI, Center for Network Science, Dept of Physics, Biology and Computer Science, Northeastern University, NICHOLAS CHRISTAKIS, Dept of Health Care Policy, Harvard Medical School — We study the evolution of patient illness using a network summarizing the disease associations extracted from 32 million Medicare claims recorded from 13 million elders using the ICD9-CM format. We find that the evolution of patients’ illness is accurately described by a process in which once a patient develops a particular disease, subsequent disease are seen to occur among diseases lying close by in the network. In addition, we find that patients affected with diseases with high network connectivity are more likely to die during a follow-up period of eight years.

9:00AM P39.00006 Bilateral interactions in disease dynamics - Decreasing epidemic thresholds with facilitated contact rates, ALEJANDRO MORALES GALLARDO, MPI-DS, Gottingen, DIRK BROCKMANN, Northwestern University, Evanston, THEO GEISEL, University of Gottingen, MPI-DS, Gottingen — Compartmental epidemiological models are very successful modeling paradigms in epidemiology. Typically, they are employed for quantitative assessments of key parameters such as the basic reproduction number $R_0$. These models rest on two key assumptions: 1.) a population is well mixed 2.) transmission is triggered by a population averaged contact rate. However, experimental evidence shows that contact rates vary substantially, and it has been hypothesized that this variability can change the dynamics of population relevant disease dynamics. However, for inhomogeneous populations the translation of distributed contact rates into effective disease transmission events is non-trivial. Transmission may either depend only on the contact rate of the transmitting individual alone (unilateral transmission), or on the contact rates of transmitting and receiving individual (bilateral transmission). In the SIS model we show that in either systems the endemic state of a disease can be stable for values of $R_0 < 1$ unlike homogeneous systems with a critical value $R_0 = 1$. Furthermore, bilateral contact dynamics entail parameter regimes in which a stable endemic state can cease to exist if the mean contact rate is increased, an unexpected effect absent in homogeneous populations.

9:12AM P39.00007 Single species victory in a two-site, two-species model of population dispersion, JACK WADDELL, Department of Computer Science, University of Michigan, Ann Arbor, Michigan 48109-1043, LEN SANDER, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109-1120, DAVID KESSLER, Department of Physics, Bar-Ilan University, Ramat-Gan ILS9200, Israel — We study the behavior of two species, differentiated only by their dispersal rates in an environment providing heterogeneous growth rates. Previous deterministic studies have shown that the slower-dispersal species always drives the faster species to extinction, while stochastic studies show that the opposite case can occur given small enough population and spatial heterogeneity. Other models of similar systems demonstrate the existence of an optimum dispersal rate, suggesting that distinguishing the species as faster or slower is insufficient. We here study the interface of these models for a small spatial system and determine the conditions of stability for a single species outcome.

9:24AM P39.00008 Color Triads in Complex Networks: Uncovering Racial Segregation Patterns in US High Schools, JULIAN CANDIA, MARTA GONZALEZ, Northeastern University — Introducing color subgraph analysis as a novel tool for characterizing complex network structures, we identify the basic racial patterns in a nationally representative sample of all public and private High Schools in the US. We apply this method on color triad subgraphs and obtain quantitative measurements on racial homophily effects, as well as on inter racial mixing patterns. Strongest homophily phenomena are observed within the white student population, followed in decreasing order by black, hispanic and asian students. Racial reciprocity measurements reveal that white students tend to form triads in which they constitute a racial majority. Black-hispanic triads are also observed to be non-reciprocal, while black-asian and hispanic-asian triads show a stronger tendency towards symmetric ties. Racial preference measurements show a rather weak white-black affinity. Since both white and black triad majorities prefer a hispanic third party, hispanic students may play the role of a bridge between white and black students. In order to design better integration strategies, quantitative observations on homophily and interracial mixing patterns could be used to redefine school organizational features. Moreover, the color subgraph analysis method can be applied to a large variety of complex network systems on other interdisciplinary fields of science.

9:36AM P39.00009 A Bayesian approach to network modularity, JAKE HOFMAN, Columbia University, Department of Physics, CHRIS WIGGINS, Columbia University, Department of Applied Mathematics and Applied Physics — We present an efficient, principled, and interpretable technique for inferring module assignments and identifying the optimal number of modules in a given network. Our approach is based on a probabilistic network model equivalent to an infinite-range spin-glass Potts model on the irregular lattice defined by a given network; the problem of identifying modules is then tantamount to inferring distributions over both the module assignments (i.e. spin states) and the model parameters (i.e. coupling constants) while also identifying the number of modules (i.e. number of occupied spin states) in the network. Using a variational approximation we derive a mean-field free energy, the minimization of which provides controlled approximations to the distributions of interest. We show how several existing methods for finding modules can be described as variant, special, or limiting cases of our work, and how related methods for complexity control — identification of the true number of modules — are outperformed. We apply the technique to synthetic and real networks and outline how the method naturally allows selection among competing network models.

9:48AM P39.00010 Distribution of Node Characteristics in Complex Networks, JULYONG PARK, A.-L. BARABASI, Northeastern University — Our enhanced ability to map the structure of various complex networks is accompanied by the capability to independently identify the functional characteristics of each node, leading to the observation that nodes with similar characteristics show tendencies to link to each other. Examples can be easily found in biological, technological, and social networks. Here we propose a tool to quantify the interplay between node properties and the structure of the underlying network. We show that when nodes in a network belong to two distinct classes, two independent parameters are needed. We find that the network structure limits the values of these parameters, requiring a phase diagram to uniquely characterize the configurations available to the system. The phase diagram shows independence from the network size, a finding that allows us to estimate its shape for large networks.

1 supported by the James McDonell Foundation, NSF, NIH, and NORT


10:00AM P39.00011 The Modular Structure of Protein Networks, HERNAN D. ROZENFELD, DIEGO RYBSKI, Levich Institute, City College of New York, New York 10031, USA, SHLOMO HAVLIN, Minerva Center and Department of Physics, Bar-Ilan University, 52900 Ramat-Gan, Israel, HERNAN A. MAKSE, Levich Institute, City College of New York, New York 10031, USA — The evolution of the human protein homology network (H-PHN) has led to a complex network that exhibits a surprisingly high level of modularity. Topologically, the H-PHN presents well connected groups (conformed by proteins of similar aminoacid structure) and weak connectivities between the groups. Here, we perform an empirical study of the H-PHN to characterize the degree of modularity in terms of scale-invariant laws using recently introduced box covering algorithms. We find that the exponent that gives insight into the evolutionary process that led to the modular organization and dynamics of the present H-PHN.
10:12AM P39.00012 Synchronization behavior in linear arrays of negative differential resistance circuit elements, HUIDONG XU, STEPHEN TEITSWORTH, Duke University — We study the electronic transport properties in a linear array of nonlinear circuit elements that exhibit negative differential resistance, and find that state-cluster synchronization emerges when there is heterogeneity in the element properties. This type of synchronization is associated with a non-uniform spatial distribution of total applied voltage across the array elements, as well as the formation of multiple stable branches in computed current-voltage curves for the entire array. Unlike most synchronizing systems studied previously [1], this system possesses coupling between elements that displays both positive and negative feedback depending on the state of each element. An empirical order parameter is defined which quantifies the degree of synchronization. We also find that the degree of synchronization is strongly dependent on the ramping rate of the total applied voltage to the array, with complete synchronization observed in the limit of small ramping rate. This model provides a basis for describing related nonlinear phenomena in more complex electronic structures such as semiconductor superlattices [2]. [1] A. Pikovsky, M. Rosenbaum, and Jürgen Kurths, Synchronization: a universal concept in nonlinear sciences (Cambridge University Press, Cambridge, 2001). [2] M. Rogozia, S. W. Teitsworth, H. T Grahn, and K. H. Ploog, Phys. Rev. B65, 205303 (2002).

10:24AM P39.00013 Hierarchical, 4-connected Small-World Graph1, BRUNO GONCALVES, STEFAN BOETTCHER, Emory University — A new sequences of graphs are introduced that mimic small-world properties. The graphs are recursively constructed but retain a fixed, regular degree. They consist of a one-dimensional lattice backbone overlaid by a hierarchical sequence of long-distance links in a pattern reminiscent of the tower-of-hanoi sequence. These 4-regular graphs are non-planar, have a diameter growing as $2\sqrt{\ln N}$ or as $(\log N)^\alpha$ with $\alpha \sim (\log_2 N + \log_2 \log_2 N^2)$, and a nontrivial phase transition $T_c > 0$, for the Ising ferromagnet. These results suggest that these graphs are similar to small-world graphs with mean-field-like properties.

1Division of Materials Research at the NSF, grant #0312150

10:36AM P39.00014 Exact Renormalization of Super-Diffusion on the Tower-of-Hanoi Network, STEFAN BOETTCHER1, BRUNO GONCALVES2, Physics Department, Emory University — We propose the Tower-of-Hanoi network as a hierarchical, small-world network possessing both, geometric and long-range links. Modeling diffusion via a random walk on this network provides a mean-square displacement $\sqrt{\ln(2)} = 1.30576$. Here, $\phi = (1 + \sqrt{5})/2$ is the “golden ratio” that is intimately related to Fibonacci sequences. This may be the first solvable model with super-diffusion for any fractal structure. This appears to be also the first known instance of any physical exponent containing $\phi$. It originates from an unusual renormalization group fixed point with a subtle boundary layer. The connection between network geometry and the emergence of $\phi$ in this context is still elusive.

1http://www.physics.emory.edu/faculty/boettcher/
2http://www.bgoncalves.com/

10:48AM P39.00015 Scaling behavior of the non-affine deformation of random fiber networks, HAMED HATAMI-MARBINI, CATALIN PICU, Rensselaer Polytechnic Institute — Random fiber networks exhibit non-affine deformation on multiple scales. This controls to a large extent their “homogenized” behavior on the macroscopic (system level) scale. It is currently believed that denser networks and networks in which the fibers have vanishing bending stiffness deform affinely. Here we show that these conclusions depend on the nature of the measure used to probe the non-affine. If a strain based measure is used, it can be shown that all networks, irrespective of the axial or bending behavior of their fibers are non-affine. Furthermore, the non-affinity decreases with the observation scale, exhibiting a universal power law scaling. The behavior of dense and sparse networks is shown to be similar if a scale renormalization is applied.

Wednesday, March 12, 2008 8:00AM - 10:48AM —
Session P40 DCMP: Surface Effects, Thermodynamics and Fabrication Morial Convention Center 232

8:00AM P40.00001 Surface core-level shifts and atomic coordination at the W(320) surface, XUBING ZHOU, J.L. ERSKINE, Department of Physics, University of Texas at Austin, O. KIZILKAYA, Center for Advanced Microstructures and Devices — High resolution 4f core-level photoemission spectra are reported from the W(110) and from the related vicinal W(320) surfaces. Curve fittings of the spectra permit tests of core-level binding-energy shift models that relate local atomic coordination to binding –energy differences associated with (for example) terrace and step-edge atoms. A well-resolved shoulder on the W(320) surface peak is attributed to step-edge atoms and contributions from surface atoms having higher atomic coordination are obtained from the curve-fitting exercises. The results are discussed in relation to prior core-level measurements, tight-binding models, and ab-initio calculations of core-level shifts for W(320).

1This work was supported by The Rebert A Welch Foundation.

10:12AM P40.00002 Secondary electron spectra of Au and Cu under bombardment by very low energy positrons, S. MUKHERJEE, A.H. WEISS, M.P. NADESLINGAM, U. Texas at Arlington, P. GUAGLIARDO, A. SERGEANT, J. WILLIAMS, U. Western Australia — Measurements of the secondary electron energy spectra resulting from very low energy positron bombardment of a polycrystalline Au and Cu (100) surfaces are presented. The low energy part of the secondary spectra contain significant contributions from two processes: 1. annihilation induced Auger electrons that have lost energy before leaving the surface and 2. secondary electrons resulting from direct energy exchange with an incident positron. Our data indicate that the second process (direct energy exchange with the primary positron) is still important at and below 3 eV incident beam energy. Since energy conservation precludes secondary electron generation below an incident beam energy equal to the difference between the electron and positron work functions (~3eV), the fact that we still observe significant secondary electron emission at energies at or below this value provides strong evidence that the incident positrons are falling directly into the surface state and transferring all of the energy difference to an outgoing secondary electron.

1Y-1100 Welch Foundation
8:24AM P40.00003 Fermi-liquid effects in propagation of low frequency electromagnetic waves through thin metal films\(^1\). NATALYA ZIMBOVSKAYA, GRIGORY ZIMBOSKIY, University of Puerto Rico-Humacao — In the present work we theoretically analyze the contribution from a transverse Fermi-liquid collective mode to the transmission of electromagnetic waves through a thin film of a clean metal in the presence of a strong external magnetic field. We show that at the appropriate Fermi surface geometry the transverse Fermi-liquid wave may appear in conduction electrons liquid at frequencies \( \omega \) significantly smaller than the cyclotron frequency of charge carriers \( \Omega \) provided that the mean collision frequency \( \tau^{-1} \) is smaller than \( \omega \). Also, we show that in realistic metals size oscillations in the transmission coefficient associated with the Fermi-liquid mode may be observable in experiments. Under certain conditions these oscillations may predominate over the remaining size effects in the transmission coefficient.

\(^1\)This work was supported by DoD grant W911NF-06-1-0519

8:36AM P40.00004 Ground-state structure of the hydrogen double vacancy on Pd(111). SUNGHO KIM, SEONG-GON KIM, Mississippi State University, STEVEN ERWIN, Naval Research Laboratory — We determine the ground-state structure of a double vacancy in a hydrogen monolayer on the Pd(111) surface. We represent the double vacancy as a triple vacancy containing one additional hydrogen atom. The potential-energy surface for a hydrogen atom moving in the triple vacancy is obtained by density-functional theory, and the wave function of the fully quantum hydrogen atom is obtained by solving the Schrödinger equation. We find that an H atom in a divacancy defect experiences significant quantum effects, and that the ground-state wave function is centered at the hcp site rather than the fcc site normally occupied by H atoms on Pd(111). Our results agree well with scanning tunneling microscopy images.

8:48AM P40.00005 Band Mapping in Higher-Energy X-Ray Photoemission: Phonon Effects and Comparison to One-Step Theory. JAN MINAR and Comparison to One-Step Theory. JAN MINAR, Ludwig Maximilian University, Munich, LUKASZ PLUCINSKI, IFF-9, Research Center Juelich, BRIAN SELL, Otterbein College, Westerville, Ohio, JUERGEN BRAUN, Hildesheim University, HUBERT EBERT, Ludwig Maximilian University, Munich, CLAUS SCHNEIDER, IFF-9, Juelich Research Center, CHARLES FADLEY, UC Davis and LBNL. Mat. Sc. Div. — In view of the present interest in more bulk sensitive band mapping via x-ray photoemission, we have studied the temperature dependence of W(110) angle-resolved spectra excited at photon energies of 260, 870 eV, and 1254 eV and between 300K and 780K. Experimental results are compared to both a free-electron final-state model and theoretical one-step model calculations. At 300K, clear band dispersions can be observed in the data. The ratio between direct and non-direct transitions is approximately estimated from a Debye-Waller factor. One-step theoretical calculations reproduce well band dispersions and matrix element effects in the measured spectra at room temperature, but including phonon effects via complex phase shifts does not predict density-of-states related features observed in higher-temperature spectra. We will also discuss the implications of this work for future experiments on other materials and at even higher photon energies up to 10 keV.

9:00AM P40.00006 Electronic Gr"uneisen Parameter In Paramagnetic Nickel\(^1\). SHOUHUA NIE, XUAN WANG, JUNJIE LI, RICHARD CLINITE, MARK WARTENBE, JIANMING CAO, Physics Department and National High Magnetic Field Laboratory, Florida State University — We have conducted the first measurement of electronic Gr"uneisen parameter \(\gamma_e\) in the paramagnetic state of ferromagnetic transition metal nickel by monitoring the laser-induced ultrafast stress dynamics using femtosecond electron diffraction. This method overcomes the restriction of traditional low-temperature methods and offers a unique path to study electronic thermal expansion in magnetic metals. Our measurement indicates that the local magnetic moment that persists in the paramagnetic state of nickel does not contribute significantly to electronic thermal expansion. This result would serve as an important test of current models regarding the magnetism in ferromagnetic transition metals.

\(^1\)Physics Department and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310

9:12AM P40.00007 Generalized Surface Thermodynamics of Solids with Application to Nucleation\(^1\). ROBERT CAMMARATA, Johns Hopkins University — J.W. Gibbs formulated a general thermodynamics for surfaces in multicomponent fluid systems. For the case of solid-fluid surfaces, he restricted attention to single component solids. Attempts to generalize Gibbs’ results for surfaces between multicomponent solids and fluids are problematic owing to the difficulty that the surface chemical potentials in the solid are generally not well defined, and therefore any expressions involving these chemical potentials will also not be well defined. A formulation of a general surface thermodynamics that can take into account capillary effects in systems involving interfaces between multicomponent solids and fluids while avoiding the aforementioned difficulties will be discussed that utilizes the concept of thermodynamic availability. It will be shown how this approach allows Gibbs-Thomson effects for finite size solids, an adsorption equation for a solid surface, and the thermodynamics of nucleation during solidification to be treated in a straightforward manner that avoids all references to ill defined surface quantities. In particular, a derivation will be presented that is the first to properly generalize Gibbs’ analysis for the reversible work of nucleation to the case of solidification.

\(^1\)Support from the National Science Foundation under grant number DMR 0706178.

9:24AM P40.00008 Controlling precipitate growth in aluminum rich alloys via externally applied stress\(^1\). JACK FRANKLIN, JENNIFER LUKES, University of Pennsylvania — The material properties of metallic alloys are directly influenced by their microstructure. The final microstructure of bulk specimens is currently determined through specific heat treatments designed to control the homogenous precipitation of secondary phases from a saturated matrix. This talk will introduce a novel stress-based method of controlling the precipitation and directed growth of secondary phases to create desired microstructures on the surface of an aluminum-copper alloy. Microstructures obtained under different stress conditions will be presented and the mechanisms leading to their formation will be discussed.

\(^1\)This work is supported by the National Science Foundation (CBET-0404259)

9:36AM P40.00009 Bulk nanostructured alloys by large strain extrusion machining. WILFREDO MOSCOSO, CHRISTOPHER SALDANA, JON MADARIAGA, Purdue University, RAVI SHANKAR, University of Pittsburgh, SRINIVASAN CHANDRASEKAR, DALE COMPTON, Purdue University — Large strain extrusion machining (LESM) is presented as a method of severe plastic deformation for the creation of bulk nanostructured materials in a wide range of metal alloys. This method combines inherent advantages afforded by large strain deformation in chip formation by machining, with simultaneous dimensional control of extrusion in a single step of deformation. Bulk nanostructured materials in the form of foils, plates, and bars of controlled dimensions are shown to result by appropriately controlling the geometric parameters of the deformation in large strain extrusion machining.
9:48AM P40.00010 Engineering materials-design parameters of the Mg-Li Alloy System from ab initio calculations, WILLIAM COUNTS, MARTIN FRIAK, DIERK RAABE, JORG NEUGEBAUER, Max-Planck Institute for Iron Research — Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. Fundamental physical properties (like formation energy and elastic constants) of 11 bcc magnesium-lithium alloys were calculated using density-functional theory (DFT) and compared with available experimental data. These DFT determined properties were in turn used to calculate engineering properties like the bulk modulus/shear modulus (B/G) and Young’s modulus/density (E/ρ). From these engineering parameters, alloys with optimal mechanical properties need for a light weight structural material were identified. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% magnesium while the most ductile alloys have 0-20 at.% magnesium. In addition, the specific modulus for alloys with 70 at.% magnesium was found to be equal to that of aluminum-magnesium alloys and slightly lower than that of aluminum-lithium alloys.

10:00AM P40.00011 Testing the MacPherson-Srolovitz Theory in Simulations of 3D Grain Growth, ANTHONY ROLLETT, FATMA UYAR, SETH WILSON, JASON GRUBER, SUKBIN LEE, Carnegie Mellon University — The theory by MacPherson and Srolovitz provides an exact prediction of the growth rate of individual cells or grains in a space-filling network (microstructure). Testing the predictions of the theory requires measurement of mean width and edge lengths where three cells meet at triple line junctions. This is most easily accomplished in networks that are discretized with a mesh. A Moving Finite Element (MFE) model was used to simulate the evolution (growth) over short times of a network discretized on a tetrahedral mesh and growth rates. Volumes, mean widths and edge lengths were measured. The growth rates measured from the simulation were found to be in very good agreement with the predictions of the MacPherson-Srolovitz theory. The results from similar measurements in Monte Carlo and Phase Field models of grain growth will also be reported. In this case, measurement of mean width and edge length is complicated by use of a regular grid to discretize the network on a set of points or voxels. A modified algorithm by Ohser and Mücklich is used to measure mean width. Edge length measurement along triple lines requires conversion of the voxel image to a surface mesh.

10:12AM P40.00012 Phase-field Simulation for Analyzing Time Evolution of Grains of Precipitate in Phase Decomposition Processes of Magnetic Alloys, YOSHIHARU KANEGAI, Mechanical Engineering Research Laboratory, Hitachi, Ltd. — The time evolution of the average grain size and the number of grains of precipitate in phase decomposition processes of magnetic alloys in two-dimensional systems was investigated using phase-field simulation. Specifically, the phase decomposition processes of Fe-Cu and Fe-Cr systems were studied. Chemical free energy from a thermodynamic database of phase diagrams was used and magnetic contribution was considered. In appropriate compositions, these systems show spinodal decomposition followed by Ostwald ripening. In the long-time region of these processes, the time evolution of the average grain size and the number of grains of precipitate was evaluated by the power of time. The exponent of the power of time of the average grain size was $\alpha \sim 1/3$, consistent with the Lifshitz-Slyozov-Wagner theory. On the other hand, that of the number of grains $\beta$ was $\beta \sim 2/3$, inconsistent with the theory, which predicts $\beta \sim 1$. However, it was shown that in two-dimensional systems these results are reasonable.

10:24AM P40.00013 Modeling Digestive and Ostwald Ripening of Nanocrystals, MICHAEL TAMBASHCO, Columbia University, SANAT KUMAR — Ostwald and digestive ripening are two diametrically opposite phenomena that dramatically impact nanocrystal polydispersity. Ostwald ripening allows for large nanocrystals to grow at the expense of small ones, while digestive ripening involves the propulsion of small nanocrystals. Chemical free energy from a thermodynamic database of phase diagrams was used and magnetic contribution was considered. Chemical free energy from a thermodynamic database of phase diagrams was used and magnetic contribution was considered. In appropriate compositions, these systems show spinodal decomposition followed by Ostwald ripening. In the long-time region of these processes, the time evolution of the average grain size and the number of grains of precipitate was evaluated by the power of time. The exponent of the power of time of the average grain size $\alpha$ was $\alpha \sim 1/3$, consistent with the Lifshitz-Slyozov-Wagner theory. On the other hand, that of the number of grains $\beta$ was $\beta \sim 2/3$, inconsistent with the theory, which predicts $\beta \sim 1$. However, it was shown that in two-dimensional systems these results are reasonable.

10:36AM P40.00014 Mean-field Theory of Multicomponent Phase Coarsening, KE-GANG WANG, Department of Physics and Space Sciences, Florida Institute of Technology — Study of phase coarsening in multicomponent systems is rare. Morral and Purdy developed a general theoretical frame for phase coarsening in n-component alloys. However, all work considered only the effect of solution thermodynamics, and ignored the kinetic effect from non-zero volume fraction. Therefore, all studies are valid only in the case of vanishing volume fraction. When $V_{f}$ is not zero, the interactions among precipitates exist. The diffusion screening length is used to describe these interactions, and it is found that the growth rate of particle depends on the volume fraction through diffusion screening length. A mean-field theory of multicomponent phase coarsening will be presented, which includes effects of both multicomponent thermodynamics and kinetics from nonzero volume fraction.

Wednesday, March 12, 2008 11:15AM - 1:39PM — Session Q1 DCMP: Ballistic Charge and Spin Transport in Graphene Morial Convention Center LaLouisiane AB

11:15AM Q1.00001 Electronic spin transport and spin precession in single graphene layers at room temperature, BART VAN WEES, University of Groningen — I will give a review of our experiments on spin injection, spin transport and spin precession in field effect transistors based on single graphene layers. We have employed a four terminal non-local measurement technique which allows us to fully separate the electronic charge and spin circuits. One pair of ferromagnetic electrodes is used as spin injectors, the other pair as spin detectors. By using different widths for the ferromagnetic electrodes we are able to control the coercive fields and prepare the magnetization direction of each with an applied magnetic field (in positive or negative x-direction). We observe clear signals due to spin diffusion from injector to detector electrodes. From the dependence of the spin signals on electrode spacing we obtain a spin relaxation length of 1.5 to 2 micrometer, and a corresponding spin relaxation time of about 100 ps [1]. These measurements are confirmed by Hanle-type spin precession measurements where the injected spins precess around a magnetic field applied perpendicular to the graphene plane. The spin signals only weakly depend on temperature (between 4.2 K and 300K), and also change little when the gate voltage is tuned from the metallic electron/hole regimes to the Dirac neutrality point. Recent experiments show that the spin relaxation times/lengths are similar for spin directions pointing in the graphene plane and perpendicular to the graphene plane [2]. Also the presence of an Al$_2$O$_3$ layer on top of the graphene does not significantly change the spin relaxation length and time. I will discuss these results in the light of existing theories for spin-orbit interaction in graphene. The implications for graphene spintronics and graphene qubits will be discussed.

11:15AM Q1.00002 Phase coherent transport in graphene, ALBERTO MORPURGO, Delft University — The investigation of transport phenomena originating from quantum interference of electronic waves has proven to be a very effective probe of the electronic properties of conducting materials. Recent work has shown that this is also the case for graphene, a novel material consisting of an individual layer of carbon atoms, in which the electronic dynamics is governed by the Dirac equation. After introducing the peculiar aspect of the low-energy electronic properties of graphene that are important to understand quantum interference in this material, I will present our experimental work. I will first discuss our study of Aharonov-Bohm conductance interference in single- and bi-layer graphene devices, we show that the minimum conductivity value is geometry dependent and approaches the theoretical value of $4e^2/h$ only for wide and short graphene strips. Moreover, we observe periodic conductance oscillations with bias and gate voltages, arising from quantum interference of multiply-reflected waves of charges in graphene. When graphene is coupled to superconducting electrodes, we observe gate tunable supercurrent and sub-gap structures, which originate from multiple Andreev reflection at the graphene-superconductor interfaces. Our results demonstrate that graphene can act as a quantum billiard with a long phase coherence length. *This work was supported in part by DOD/DMEA-H94003-06-2-0608.*

1:03PM Q1.00004 Ballistic Transport in Graphene,1 MIKHAIL TITOV, Heriot-Watt University, Edinburgh — Charge transport in ballistic graphene-based microstructures is described within the scattering formalism, which takes into account evanescent modes induced by metallic contacts. We discuss in detail new theoretical predictions for the charge transport and shot noise in the models which include local potential inhomogeneities, next to the nearest neighbor coupling, or ripples in the graphene plane.

1 Support from the School of Engineering and Physical Sciences at Heriot-Watt University is gratefully acknowledged.

**Wednesday, March 12, 2008 11:15AM - 2:15PM**

Session Q2 DBP DMP: The Physics of Self-Assembled Protein Cages

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11:15AM Q2.00001 Packaging of Polyelectrolytes in Viral Capsids: The Interplay Between Polymer Length and Capsid Size1, CHARLES KNOBLER, UCLA, Dept. of Chemistry and Biochemistry — Each particle of the Cowpea Chlorotic Mottle Virus (CCMV) has a very small “parts list,” consisting of two components: a molecule of single-stranded RNA and a 190-residue protein that makes up the 28-nm diameter capsid. When purified viral RNA and capsid protein are mixed in solution at an appropriate pH and ionic strength, infectious wild-type viruses form spontaneously. Virus-like particles (VLPs) are formed when the protein self-assembles around other anionic polymers such as poly(styrene sulfonate) (PSS). Under different pH and ionic strength conditions the capsid protein can assemble by itself into empty capsids, multishell structures, tubes and sheets. To explore the effect on virion size of the competition between the preferred curvature of the protein and the size of the packaged cargo we have examined the formation of VLPs around PSS polymers with molecular weights ranging from 400 kDa to 3.4 MDa. Two distinct sizes are observed — 22 nm for the lower molecular weights, jumping to 27 nm at 2 MDa. While under given conditions the size of PSS in solution is directly determined by its molecular weight, the self-complementarity of RNA makes its solution structure dependent on the nucleotide sequence as well. We have therefore employed Small-Angle X-ray Scattering and Fluorescence Correlation Spectroscopy to examine the sizes of viral and non-viral RNAs of identical lengths. A model for the assembly that includes both the inter-self interactions of the polyelectrolyte and the capsid proteins and the interactions between them provides insight into the experimental results.

1 This work was supported by National Science Foundation Grant CHE-0400363

11:51AM Q2.00002 Diversity in virus assembly: biology makes things complicated, ADAM ZLOT-NICK, Biochemistry & Molecular Biology, OUHSC — Icosahedral viruses have an elegance of geometry that implies a general path of assembly. However, structure alone provides insufficient information. Cowpea Chlorotic Mottle Virus (CCMV), an important system for studying virus assembly, consists of 90 coat protein (CP) homodimers condensed around an RNA genome. The crystal structure (Speir et al, 1995) reveals that assembly causes burial of hydrophobic surface and formation of $\beta$ hexamers, the intertwining of N-termini of the CPs surrounding a quasi-sixfold. This structural view leads to reasonable and erroneous predictions: (i) CCMV capsids are extremely stable, and (ii) $\beta$ hexamer formation is critical to assembly. Experimentally, we have found that capsids are based on a network of extremely weak (4-5 kT) pairwise interactions and that pentamer formation is the critical step in assembly kinetics. Because of the fragility of CP-Cp interaction, we can redirect assembly to generate and dissociate tubular nanostructures. The dynamic behavior of CCMV reflects the requirements and peculiarities of an evolved biological system; it does not necessarily reflect the behavior predicted from a more static picture of the virus.

12:27PM Q2.00003 Dynamic Models for Templated Viral Capsid Assembly, MICHAEL HAGAN, Physics Department, Brandeis University — The replication of many viruses with single-stranded genomes requires the simultaneous assembly of an ordered protein shell, or capsid, and encapsidation of the genome. In this talk, I will present coarse-grained computational and theoretical models that describe the assembly of viral capsid proteins around interior cores, such as polymers and rigid spheres. These models are motivated by two recently developed experimental model systems in which viral proteins dynamically encapsidate inorganic nanoparticles and polyelectrolytes. Model predictions suggest that some forms of cooperative interactions between subunits and cores can dramatically enhance rates and robustness of assembly, as compared to the spontaneous assembly of subunits into empty capsids. For large core-subunit interactions, subunits adsorb onto a core en masse in a disordered manner, and then undergo a cooperative rearrangement into an ordered capsid structure. These assembly pathways are unlike any seen for empty capsids formation. While model predictions suggest that cooperative interactions between disparate assembling components can overcome some limitations of spontaneous assembly, the complexity of multicomponent assembly introduces new forms of kinetic traps that can frustrate assembly, and hence introduces new limitations. These findings have implications for a mechanism in which viruses use interactions between proteins and genomic molecules to promote and control assembly, and thereby control the replication process.

1:03PM Q2.00004 Self-Assembly of the HIV Virus, ROBINN BRUINSMA, University of California, Los Angeles — The talk will discuss the application of the continuum theory of elastic shells to understand the different morphologies of Retroviral capsids. Minor differences in molecular structure between different capsid proteins produce large changes in capsid morphology. Continuum elasticity theory can account for the capsid shape “phase-diagram.” The conical shape of the capsid of the HIV virus is the result of assembly “constraints” in the form of the enclosing lipid bilayer and the osmotic pressure of the encapsidated genome molecules.
11:15AM Q3.00001 Quasielastic scattering – theory and experiment hand in hand, JULIA HIGGINS, Imperial College, London — In his early career de Gennes worked with colleagues at the CEA Saclay and was familiar with the new possibilities offered for studying materials using neutron scattering techniques. He published a number of papers in this field, two of the most influential being in the field of polymer dynamics where he developed theoretical descriptions of quasi-elastic scattering from single polymer chains in solution. The first results were based on the Rouse model of a polymer chain with no dynamic interaction with the solvent. The second paper appearing a few years later extended the theory to take account of hydrodynamic interactions with the solvent (the so-called Zimm model). These papers appeared at the time when high resolution quasi-elastic scattering techniques were being developed at a number of neutron sources and were influential in driving some of the first experimental investigations of polymer dynamics using neutrons. As dynamic light scattering developed, particularly from large biological molecules the theory was also applied here. The subsequent development of the reptation model for polymer molecules in the dense phase, and the publication by de Gennes of the scattering law expected from a reptating chain also coincided with developments in experimental techniques, in particular the neutron spin-echo technique. This technique allowed the scattering from single polymer molecules in dense phases to be observed and provided some of the first direct experimental tests of the reptation model. Quasielastic scattering and particularly neutron spin-echo techniques have been continually developing in subsequent decades, and both local side group dynamics and main chain motion have been investigated in detail, as well as collective motions in these glass forming materials. Interpretation of the data has been considerably advanced by the parallel development of modelling, particularly molecular dynamic simulations. New neutron sources with even higher fluxes currently being commissioned include QENS in their portfolio of instruments so that we can anticipate further experimental investigation of polymer dynamics, to compare to ever more sophisticated modelling.

11:51AM Q3.00002 The Coil-Stretch Transition after more than 30 years, ERIC SHAQFEH, Stanford University — From the seminal paper of DeGennes (1974), there has been a long debate over the nature of polymer dynamics surrounding the “critical point” in flow strength where local fluid line extension rates (and the resulting drag created on a linear polymer) dominate over the entropic restoring force – the so-called coil-stretch transition. This debate has now essentially ended as a result of recent single molecule experiments and large scale molecular simulations which demonstrate that, for steady extensional flow, the basic tenets DeGennes put forth were correct, albeit with certain details which DeGennes did not foresee. However, for flows which are either not steady or which contain significant vorticity, there are qualitatively different features which have now been suggested and remain essential to understand. For example, molecular simulations of planar mixed flows demonstrate that conformational fluctuations play a key role in the coil-stretch transition especially for flows that are “near shear”. Finally, the application of the DeGennes’ ideas to turbulent drag reduction are far from clear, and new large scale molecular simulations have shed some light on polymer dynamics in this important application.

12:27PM Q3.00003 Dynamics of Polymer Solutions, WILLIAM GRAESSLEY, Princeton University — No abstract available.

1:03PM Q3.00004 Dynamics of Entangled Polymers, MICHAEL RUBINSTEIN. University of North Carolina — The effect of entanglements on polymer dynamics is one of the most interesting and most challenging areas of polymer physics. In 1967 Edwards introduced the confining tube model for polymer networks in which the effect of permanent entanglements from surrounding chains on a given one was replaced by the confining tube potential. In 1971 de Gennes proposed reptation model, suggesting that entangled chains diffuse along their confining tubes. This ingenious idea provided a simple explanation for strong molecular weight dependence of relaxation time and self-diffusion coefficient of entangled linear polymers. In 1975 de Gennes put forward the concept of constraint release that takes into account modifications of the confining tube caused by the motion of surrounding chains forming this tube. In the same paper de Gennes showed that dynamics of entangled branched polymers, such as stars, is qualitatively different from that of entangled linear polymers. Branch points do not allow these molecules to reptate along their confining tubes, as linear molecules do, but instead stars can only relax and move by a highly entropically unfavorable process of arm retraction. I will describe the development and modification of ideas put forward in de Gennes’ original models of dynamics of entangled linear and branched polymers. Some details of de Gennes’ constraint release model were modified and the concept of tube dilation was introduced couple of years later. For the following quarter of century scientists are debating whether constraint release or tube dilation is the dominant mechanism for relaxation of branched and linear polymers. The shape of the entropic potential for the arm retraction mechanism of branched polymers proposed by de Gennes was modified by Doi and Kuzuu in 1980. This potential is acting along the primitive path – the axis of the confining tube, and the resulting relaxation time of the branched polymers strongly depends on the precise definition of this primitive path. Unfortunately, the primitive path is still not clearly defined by any of the existing models and scientists are still arguing which definition is better. I will describe these and other challenges and open questions remaining in the field of entangled polymer dynamics.

1:39PM Q3.00005 Interdiffusion and disentanglement of polymer brushes, JACOB KLEIN, Weizmann Institute of Science — In the spirit of this symposium, I will briefly survey some of the main ideas on interdiffusion and interfacial relaxation put forward by de Gennes, then consider some recent experimental developments. A very attractive feature of the central tenets of polymer physics introduced by de Gennes is their versatility in different physical situations, so that a discussion of, for example, friction, will in a natural way involve reptation. A particular case in point concerns the relaxation of interdiffused, compressed polymer brushes undergoing shear, as when they are used as lubricating layers. Here the useful concept is, unexpectedly, that of relaxation of entangled star-branched polymers, introduced by de Gennes over 30 years ago for a totally different purpose: The main idea – and conceptually a beautifully simple one - is that in order for an entangled chain emanating from a fixed branch point to relax, it needs to retract back along its ‘tube’ and dissipate the stress by re-equilibrating in a new configuration. Compression of two polymer brushes, whether in a good solvent or in the melt, creates a model interdiffused interface, whose dynamic properties can be analyzed based on such star-branched relaxation models, and the talk will describe some recent results on these systems.

Wednesday, March 12, 2008 11:15AM - 1:39PM – Session Q4 DCMP: Pairing Fluctuations Near the Superconductor-Insulator Transition Morial Convention Center 206
11:15AM Q4.00001 Survival of superconducting correlations across the two-dimensional superconductor-insulator transition: A finite-frequency study

N. PETER ARMITAGE, The Johns Hopkins University

The complex AC conductivity of thin amorphous InO films was studied as a function of magnetic field through the nominal 2D superconductor-insulator transition. We have resolved a significant finite frequency superfluid stiffness well into the insulating regime, giving direct evidence for superconducting correlations in this insulating state. As these superconducting fluctuations are temperature independent at low temperatures, this also represents the first observations of quantum superconducting fluctuations around an insulating ground-state. A phase diagram is established that includes the superconducting state as a transition to a “Bose” insulator and an eventual crossover to a “Fermi” insulating state at high fields. We speculate on the consequences of these observations, their impact on our understanding of the insulating state, and its relevance as a prototype for the insulating states of matter that derive from superconductors.


11:51AM Q4.00002 Theory of the Nernst effect near quantum phase transitions in condensed matter, and in dyonic black holes

MARKUS MUELLER, Harvard University

We present a general hydrodynamic theory of transport in the vicinity of superfluid-insulator transitions in two spatial dimensions described by “Lorentz-invariant” quantum critical points. We allow for a weak impurity scattering rate, a magnetic field B, and a deviation in the density, ρ, from that of the insulator. We show that the frequency-dependent thermal and electric linear response functions, including the Nernst coefficient, are fully determined by a single transport coefficient (a universal electrical conductivity), the impurity scattering rate, and a few thermodynamic state variables. With reasonable estimates for the parameters, our results predict a magnetic field and temperature dependence of the Nernst signal which resembles measurements in the cuprates, including the overall magnitude. Our theory predicts a “hydrodynamic cyclotron mode” which could be observable in ultralow samples. We also discuss exact results for the zero frequency transport coefficients of a supersymmetric conformal field theory (CFT), which is solvable by the AdS/CFT correspondence, mapping the CFT to a black hole problem in 3+1 dimensional anti-de Sitter space. These exact results are found to be in full agreement with the general predictions of our hydrodynamic analysis.

[1] This work was supported by NSF grant DMR-0537077 and by the Swiss National Fund for Scientific Research under grant PA002-113151.

12:27PM Q4.00003 Observation of the Nernst signal generated by fluctuating Cooper pairs

KAMRAN BEHNIA, LPEM (CNRS - ESPCI), Paris — Long-range order is destroyed in a superconductor warmed above its critical temperature (Tc). However, amplitude fluctuations of the superconducting order parameter survive and lead to a number of well-established phenomena such as paraconductivity: an excess of charge conductivity due to the presence of short-lived Cooper pairs in the normal state. According to a theory by Usyukhin, Sondhi and Huse, these pairs generate a transverse thermoelectric (Nernst) signal. In two dimensions, the magnitude of the expected signal depends only on universal constants and the superconducting coherence length, so the theory can be unambiguously tested. In a dirty superconductor, the lifetime of Cooper pairs exceeds the elastic scattering time of normal electrons in a wide temperature range above Tc and, consequently, their Nernst response dominates the one generated by the normal electrons. We studied the Nernst effect of amorphous superconducting films of Nb51.5Si48.5 and resolved a Nernst signal, which persists deep inside the normal state. The amplitude of the observed signal is in excellent agreement with the theoretical prediction [1].


1:03PM Q4.00004 Nernst effect and diamagnetism in phase fluctuating superconductors

ASHVIN VISHWANATH, UC Berkeley — We investigate the characteristic signatures that arise when superconductivity is destroyed by thermal phase fluctuations induced by a dilute mixture of mobile vortices. We find that the Nernst effect and diamagnetic response differ significantly from Gaussian fluctuations — in particular, a much sharper decay with temperature is obtained. We predict a rapid onset of Nernst signal at a temperature that tracks the transition temperature Tc, rather than the pairing temperature. We also predict a close quantitative connection with diamagnetism — the ratio of magnetization to transverse thermoelectric conductivity αEL is proportional to the temperature over a wide range of fields. We interpret Nernst effect measurements on the underdoped cuprates in terms of a dilute vortex liquid over a broad temperature range above Tc [1]. We also introduce a new formalism to study fluctuating superconductivity that deals directly with the vortex variables. This technique allows us to analyze the effect of vortex properties such as core energy on Nernst effect and diamagnetism. [1] D. Podolsky, S. Raghu and A. Vishwanath, ‘Nernst Effect and Diamagnetism in Phase Fluctuating Superconductors’, Phys. Rev. Lett. 99, 117004 (2007)

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q5 AIP APS: Panel Discussion: How Can Industry Best Support the Innovative Research That It Needs?
Morial Convention Center R01

11:15AM Q5.00001 Leveraging R&D Resources via the Joint LLC Model

MATTHEW W. GANZ, President and CEO, HRL Laboratories, LLC — Industrial scientific research labs have become increasingly stressed in recent years by a variety of external forces. Both corporations and government funding agencies have shifted their priorities from long-term fundamental research toward projects that have a high probability of shorter-term payoff. Industrial funding has been further stressed by an increasing demand for quarterly results and fierce global competition. Industry leaders are now asking their R&D labs for “home runs and not just a solid base in the physical sciences. The end of the Cold War has also left the US without a declared enemy whose overt intention was to defeat us through a mastery of large-scale weaponry based upon exploitation of fundamental physics. This, when combined with a bona-fide need for technology gap fillers to respond to on-the-ground threats in the current Middle East conflicts, has led to diminished government emphasis on long-term research in the physical sciences. Simultaneously, the global sources of R&D spending are expanding. The dramatic growth of private equity in the technology development arena has both drawn talent from industry and changed the expectations on researchers. R&D spending in China, India and many other countries is growing significantly. Thus, in order to become relevant, industry must now keep its finger on the pulse of the hundreds of billions of dollars being invested privately and publicly around the world. HRL Laboratories, LLC in Malibu, California represents a unique and successful new business model for industrial R&D. HRL was founded by Howard Hughes in 1948 as the Hughes Research Laboratory and for more than four decades was the internal R&D lab for the Hughes Aircraft Company. After a series of mergers, acquisitions and divestitures over the past 15 years, HRL is now a stand-alone LLC that is owned jointly by General Motors and the Boeing Company. HRL, with a staff of about 300, performs R&D services for GM and Boeing as well as for government and commercial entities. The central themes to HRLs business model are innovation, value and leverage. Leveraging is key to the companies success. HRLs business model has been carefully honed to allow its parent companies to perform proprietary R&D in certain areas and joint, collaborative R&D among the LLC members in others. The intellectual property arrangements are skillfully organized so that the LLC Members receive a greater than 4:1 leverage of their research dollars in terms of the IP rights gained. This briefing will describe an overview of the current industrial research environment, HRLs business model, and challenges to future success.

11:51AM Q5.00002 The Value of Long Range R&D in the Information Technology Industry

PAUL M. HORN, Distinguished Scientist in Residence, NYU and Senior VP and Dir. of Research (retired), IBM — Examples from IBM and other IT companies will illustrate how long range physics research can be financially beneficial.
12:27PM Q5.00003 Creating Value with Long Term R&D: The life science industry. DARLENE J. S. SOLOMAN, CTO and Vice President, Agilent Technologies — Agilent Laboratories looks to the future to identify, invest and enable technologies and applications that will nurture the worlds people, environment and economies, and help ensure Agilents continuing leadership. Following a brief introduction to Agilent Technologies and Agilent Laboratories, Solomon will discuss how innovation and long-term R&D are transcending traditional boundaries. Focusing on the life sciences industry, she will discuss current trends in R&D and the importance of measurement in advancing the industry. She will describe some of the challenges that are disrupting the pharmaceutical industry where significant and sustained investment in R&D has not translated into large numbers of block-buster therapeutics. Much of this gap results from the profound complexity of biological systems. New discoveries quickly generate new questions, which in turn drive more research and necessitate new business models. Solomon will highlight examples of Agilents long-range R&D in life sciences, emphasizing the importance of physics. Shell conclude with the importance of creating sustainable value with R&D.

1:03PM Q5.00004 TBD, MARK R. PINTO, CTO and Senior VP & General Manager, Energy and Environmental Solutions, Applied Materials, Inc. — TBD

1:39PM Q5.00005 Panel Discussion: How can industry best support the innovative research that it needs? ABSTRACT APS — Four industrial physics leaders will discuss the future and value of innovative research in an industrial setting, and will share perspectives on how their companies address the challenge of supporting research operations. The speakers come from varied research settings and represent a cross-section of and scientific fields including bio-physics/life sciences, materials processing equipment, information technologies and electronics. This session includes an interactive panel discussion on overcoming the challenges and the circumstances confronting industrial R&D operations.

Wednesday, March 12, 2008 11:15AM - 2:15PM – Session Q6 GMAG: Artificial and Tunable Realizations of Spin Systems Morial Convention Center RO4

11:15AM Q6.00001 Frustration in a patterned array of nanoscale ferromagnetic islands: Artificial Spin Ice1, PETER SCHIFFER2, Dept. of Physics and Materials Research Institute, Pennsylvania State University — Geometrical frustration among spins in magnetic materials can lead to exotic low temperature states including “spin ice”, in which the local moments mimic the frustration of hydrogen ion positions in frozen water. Our group has performed extensive studies of spin ice materials, and we have developed and studied an artificial geometrically frustrated magnet which shares many of the properties of the spin ice materials. This artificial frustrated system is an array of lithographically fabricated single-domain ferromagnetic islands. The islands are arranged such that the dipolar interactions between them are analogous to those in spin ice. Images of the magnetic moments of individual elements in this correlated system allow us to study the local accommodation of frustration. We see both ice-like short range correlations and an absence of long range correlations, behavior which is very similar to the low temperature state of spin ice. We have extended these studies to include theoretical analysis of the disordered state of moments. We have also used these arrays to analyze the process of demagnetization, which is necessary to access low energy collective states in our arrays and in many other magnetic systems. Our results shed light on the nature of frustration in patterned arrays and correspondingly demonstrate that artificial frustrated magnets can provide a rich new arena in which to study the physics of frustration. References: R. F. Wang et al. (Nature 2006 and Journal of Applied Physics 2007); C. Nisoli et al. (Physical Review Letters 2007).

1This research was supported by the Army Research Office and the National Science Foundation
2In collaboration with Ruifang Wang, Cristiano Nisoli, Paul Lammert, Rafael Freitas, Jie Li, Xianglin Ke, William McConville, BJ Cooley, Nitin Samarth, Vin Crespi, Mike Lund and Chris Leighton

11:51AM Q6.00002 Artificial Kagome Spin Ice1, JOHN CUMINGS, Department of Materials Science and Engineering, University of Maryland — Recently, significant interest has emerged in fabricated systems that mimic the behavior of geometrically-frustrated materials. Here, I will present the full realization of such an artificial spin ice system on a two-dimensional kagome lattice, and I will present results obtained by directly counting individual pseudospins, demonstrating rigid adherence to the local ice rule. This adherence is maintained even when the lattice is randomized through a rigorous demagnetization process. The resulting spin configuration shows not only local ice rules and long-range disorder, but also correlations consistent with spin ice Monte Carlo calculations. Deviations in the correlation values suggest that dipolar corrections are significant in this system, as in pyrochlore spin ice. Because the pseudospins can be observed directly, the system also presents new routes for determining the entropy of such frustrated systems by direct observation, without heat-capacity background subtraction. I will also present the unique behavior of the system during magnetic reversal cycles, showing avalanche-like phenomena. Because of the simplicity of the structure and the robustness of its behavior, it serves as an ideal system for studying frustration in general, including the possible influences of controllable lattice imperfections.

1This work is supported by the NSF-MRSEC at the University of Maryland, DMR0520471 and by NSF-DMR075368

12:27PM Q6.00003 Thermodynamics and dynamics of artificial square ice and related dipolar nanoarrays. GUNNAR MOLLER, University of Cambridge — Spin ice is a geometrically frustrated magnetic phase which has attracted much attention since the discovery of rare earth pyrochlores reproducing the zero-point entropy of ice found by Pauling in the 1930’s. Square ice is a two-dimensional analogue of this phase, sharing its algebraic correlations and finite entropy at zero temperature, as well as connections to exact solutions, quantum magnetism, unusual quasiparticles such as magnetic monopoles, exotic dynamics and gauge theories. Experimental realizations of two-dimensional magnetic systems could recently be achieved using lithographic fabrication techniques and local magnetic probes to detect and manipulate individual magnetic degrees of freedom [1]. We study the frustrated dipolar arrays recently manufactured by Wang et al. [1] in order to realize the square ice model in an artificial structure. In particular, we discuss models for thermodynamics and dynamics of this system [2]. We show that an ice regime can be stabilized by small changes in the array geometry; a different magnetic state, kagome ice, can similarly be constructed. At low temperatures, the square ice regime is frustrated by a thermodynamic ordering transition, which can be chosen to be ferro- or antiferromagnetic. We argue that the arrays do not fully equilibrate experimentally, and identify a likely dynamical bottleneck.

1:03PM Q6.00004 Realizing Colloidal Artificial Ice on Arrays of Optical Traps. CYNTHIA OLSON, Department, Center for the Semiconductor Physics in Nanosctructures, Fayetteville, Arkansas 72701 — Recent clever techniques for fabricating nanosize materials, one-atomic-layer-at-a-time, have simultaneously opened a door to a fantastic adventure at the frontier of physics, chemistry, biology, and engineering. Nanosize materials simply do not behave as the bulk. Indeed, the rules that govern the growth and behavior of these tiny structures are unexplored. In this talk we will discuss our recent efforts to be the architect of their shape, size, density, and position of nanostructures and along the way, the interactions between them that lead to their optical and electrical behavior. While self-assembly is providing exciting quantum dot (QD) structures to explore, like the QD molecules shown here, it is equally exciting to try to use the rules we uncover to encourage QD formation to take a desired path. Can we understand the formation of faceted nanostructures? Can we encourage or seed dot structures to form specific arrays? Is it possible to engineer greater homogeneity of dot shape and size? Can we design both the optical and electrical behavior of either individual or arrays of nanostructures to mimic those we find in nature? In this talk we will review our progress to answer these questions and discuss the possibilities and challenges ahead. For example, we will discuss the formation of individual faceted nanostructures as well as the fabrication of a vertically and laterally ordered QD stacks forming three-dimensional QD arrays. As another example, we will discuss the importance of surfaces with high Miller indices, as a template to the formation of nanostructures as well as their potential role in determining the shape and increased size uniformity of the confined structures. Importantly, these observations lead to an even more basic question of when and why high index surfaces are stable. Indeed, we have found that in order to understand the origin of high index surfaces that form nanostructures we have to study them directly.

1:39PM Q6.00005 Ultracold atomic gases in optical lattices: mimicking condensed matter and beyond. MACIEJ LIEWENSTEIN, ICFO - Institut for Photonic Sciences — I will present a short review of the newest developments of physics of ultracold atomic gases in optical lattices. After a short introduction about possibilities offered by such systems I will describe recent progress in physics of ultracold dipolar gases (generation and engineering of metastable states), ultracold disordered gases (interplay disorder-interactions, random field induced order), and ultracold gases inside an optical resonator (overlapping Mott zones). I will comment on challenging open questions concerning preparation, manipulation and detection of such systems, as well as possible applications in quantum information and precision metrology.

Wednesday, March 12, 2008 11:15AM - 2:15PM
Session Q7 FEd: Undergraduate Nanotechnology and Materials Physics Education II
Morial Convention Center R05

11:15AM Q7.00001 The Role of Engineering Design in Materials Science and Engineering Curricula. EMILY ALLEN, San Jose State University — Undergraduate materials engineering curricula diverge from materials science curricula in two important ways. An underlying requirement is to prepare the graduates for industrial positions, so they need a good grounding in processing and statistical methods, as well as a strong set of hands-on skills in materials characterization and metrology. The other distinguishing feature of an engineering education is the focus on design rather than research. In the case of materials science and engineering, the design deliverable is often a process design, a materials selection, or a failure analysis. Some of the features of education for design include the exercise of thinking about the customer's needs, functional requirements of the product, the cost of production, and the broader context of the design project in society. These ideas can be integrated or at least introduced early in the curriculum and in many different types of courses. Materials Science and Engineering programs have the dual requirement of educating both future scientists and future engineers. Graduating baccalaureate students need to be ready for engineering practice, yet many also are being readied for graduate study and research. One aspect of this ambiguity is that research and design activities are not always as clearly differentiated as they are in other engineering programs. How can one undergraduate curriculum be successful at both? One key distinguishing element in engineering practice is engineering design. Design activities occur in many aspects of the profession and may be practiced by both scientists and engineers; however it is engineering curricula, not science curricula, that tend to explicitly focus on developing the skills and methods of design practice in students. Accredited programs within colleges of engineering are required to emphasize engineering practice and design, while still providing the necessary conceptual development of the underlying science. Current practices and emerging ideas concerned with these aspects of materials education will be presented in this talk.

11:51AM Q7.00002 What Quantum Dots Can Do For You. GREGORY SALAMO, University of Arkansas, Physics Department, Center for the Semiconductor Physics in Nanosctructures, Fayetteville, Arkansas 72701 — Recent clever techniques for fabricating nanosize materials, one-atomic-layer-at-a-time, have simultaneously opened a door to a fantastic adventure at the frontier of physics, chemistry, biology, and engineering. Nanosize materials simply do not behave as the bulk. Indeed, the rules that govern the growth and behavior of these tiny structures are unexplored. In this talk we will discuss our recent efforts to be the architect of their shape, size, density, and position of nanostructures and along the way, the interactions between them that lead to their optical and electrical behavior. While self-assembly is providing exciting quantum dot (QD) structures to explore, like the QD molecules shown here, it is equally exciting to try to use the rules we uncover to encourage QD formation to take a desired path. Can we understand the formation of faceted nanostructures? Can we encourage or seed dot structures to form specific arrays? Is it possible to engineer greater homogeneity of dot shape and size? Can we design both the optical and electrical behavior of either individual or arrays of nanostructures to mimic those we find in nature? In this talk we will review our progress to answer these questions and discuss the possibilities and challenges ahead. For example, we will discuss the formation of individual faceted nanostructures as well as the fabrication of a vertically and laterally ordered QD stacks forming three-dimensional QD arrays. As another example, we will discuss the importance of surfaces with high Miller indices, as a template to the formation of nanostructures as well as their potential role in determining the shape and increased size uniformity of the confined structures. Importantly, these observations lead to an even more basic question of when and why high index surfaces are stable. Indeed, we have found that in order to understand the origin of high index surfaces that form nanostructures we have to study them directly.

12:27PM Q7.00003 An Interdisciplinary Program in Materials Science at James Madison University. CHRIS HUGHES, James Madison University — Over the past decade a core group of faculty at James Madison University has created an interdisciplinary program in materials science that provides our students with unique courses and research experiences that augment the existing, high-quality majors in physics and astronomy, chemistry and biochemistry, geology and environmental science, mathematics and statistics, and integrated science and technology. The university started this program by creating a Center for Materials Science whose budget is directly allocated by the provost. This source of funds acts as seed money for research, support for students, and a motivating factor for each of the academic units to support the participation of their faculty in the program. Courses were created at the introductory and intermediate level that are cross-listed by the departments to encourage students to enroll in them as electives toward their majors. Furthermore, the students are encouraged to participate in undergraduate research in materials since this is the most fundamental unifying theme across the disciplines. This talk will cover some of the curricular innovations that went into the design of the program to make it successful, examples of faculty and student research and how that feeds back into the classroom, and success stories of the interactions that have developed between departments because of this program. Student outcomes and future plans to improve the program will also be discussed.
1:03PM Q7.00004 Use of clickers and sustainable reform in upper-division physics courses. MICHAEL DUBSON, University of Colorado at Boulder — At the University of Colorado at Boulder, successful reforms of our freshmen and sophomore-level physics courses are now being extended to upper-division courses, including Mechanics, Math Methods, QM, E&M, and Thermal Physics. Our course reforms include clicker questions (ConcepTests) in lecture, peer instruction, and an added emphasis on conceptual understanding and qualitative reasoning on homework assignments and exams. Student feedback has been strongly positive, and I will argue that such conceptual training improves rather than dilutes, traditional, computationally-intensive and problem-solving skills. In order for these reforms to be sustainable, reform efforts must begin with department-wide consensus and agreed-upon measures of success. I will discuss the design of good clicker questions and effective incorporation into upper-level courses, including examples from materials science. Condensed matter physics, which by nature involve intelligent use of approximation, particularly lends itself to conceptual training. I will demonstrate the use of a clicker system (made by iClicker) with audience-participation questions. Come prepared to think and interact, rather than just sit there!

1:39PM Q7.00005 Thinking like a physicist: Condensed Matter and Materials Physics in the Paradigms in Physics Curriculum at Oregon State University1, JANET TATE, Oregon State University — The Paradigms in Physics Program at Oregon State University organizes the upper-division undergraduate physics curriculum to blur traditional subdisciplinary boundaries and makes use of many interactive pedagogic techniques. Condensed matter physics and materials science content appear in many places in the early curriculum, culminating in a capstone course in solid state physics where students calculate band structure of real materials related to their research projects. A mix of analytic, computational, and research approaches are employed to include, for example, traditional topics like doping in semiconductors and modern topics like carbon nanotubes.

Wednesday, March 12, 2008 11:15AM - 2:15PM – Session Q8 DFD: Colloidal Phase Behavior Morial Convention Center R06

11:15AM Q8.00001 Studies of colloids on spherical interfaces using digital holographic microscopy. JÉRÔME FUNG, RYAN J. MCCORTY, VINOTHAN N. MANOHARAN, Harvard University, Dept. of Physics — Colloidal particles pinned to the surface of an oil droplet in water form robust equilibrium structures at low area fractions. To better understand the interactions in this system, we are studying these structures and their dynamics during quasistatic changes in the area fraction. We do so by imaging the 3D structures with fast temporal resolution using digital holographic microscopy (DHM). To keep the particles in non-density matched colloidal samples in the field of view, we have constructed a new apparatus to perform DHM under time-averaged zero gravity using a rotating stage. In DHM, we illuminate a sample with a laser beam and then magnify and digitally record the interference patterns between the scattered and unscattered light. Subsequent numerical reconstruction of the recorded 2D holograms allows 3D particle tracking with millisecond time resolution and submicron spatial resolution.

11:27AM Q8.00002 Confinement Finds a Length Scale for the Colloidal Glass Transition. KAZEM EDMOND, ERIC R. WEEKS, Emory University — We study a colloidal suspension confined between two parallel walls as a model system for glass transitions in confined geometries. We use confocal microscopy to directly observe the motion of the colloidal particles, which are slower when confined. This slower motion produces glassy behavior in a sample that is liquid-like when not confined. Our results, from a range of volume fractions, demonstrate that the maximum thickness where confinement effectively defines a length scale for a given particle volume fraction. The length scale increases as the glass transition is approached. We observe that near the glass transition particle motion is strongly spatially correlated. We investigate the relationship between the length scales of these correlations and the established confinement length scale.

11:39AM Q8.00003 Dislocation nucleation and motion observed in a 2D Yukawa triangular lattice, V. NOSENKO, S. ZHDANOV, G. MORFILL, Max-Planck-Institute for extraterrestrial Physics — Dislocation nucleation and motion were studied experimentally in a 2D Yukawa triangular lattice. Edge dislocations were created in pairs in lattice locations where the internal shear stress exceeded a threshold and then moved apart in the glide plane at a speed higher than the sound speed of shear waves. The early stage of this process is identified as a stacking fault. At a later stage, supersonically moving dislocations generated shear-wave Mach cones. The experimental system, a plasma crystal, allowed observation of this process at an atomistic (kinetic) level. We used a monolayer suspension of microspheres in a plasma, i.e., a complex plasma, which is like a colloidal suspension, but with an extremely low volume fraction and a partially-ionized rarefied gas instead of solvent. At our experimental conditions, the suspension forms a highly ordered 2D triangular lattice. Dislocations were generated in this lattice due to the shear stress introduced by its differential rotation, with two “rigid” domain walls imbedded in it. We used digital video microscopy for direct imaging and particle tracking.

11:51AM Q8.00004 Low-electric-field phase behaviour of Brownian colloidal suspensions in sedimentation equilibrium. AMIT AGARWAL, NING LI, ANDAN YETHIRAJ, Department of Physics and Physical Oceanography, Memorial University of Newfoundland — We study the phase diagram of the suspension of micron-scale fluorescent labeled silica colloids in aqueous suspension as a function of concentration in the presence of a moderate (less than 1 volt per μm) AC electric field. Confocal microscopy was used to track three-dimensional structure and dynamics of colloidal suspensions in sedimentation equilibrium. We characterize thresholds for field-induced organization in monodisperse colloidal suspensions of two particle sizes using orientational order parameters. We then study structure formation at moderate fields above the field threshold. At concentrations greater than 10%, and electric fields much larger than the field threshold measured, the colloidal suspension crystallizes to form a body centered tetragonal structure as has been previously reported. At lower concentrations and moderate fields, we uncover complex structure formation phenomena that include equilibrium cellular structures.

12:03PM Q8.00005 Benchmarks for simulations of colloidal suspensions1, TONY LADD, University of Florida — There are now a number of methods available to investigate the dynamics of colloidal suspensions; among the most popular are Stokesian dynamics, the lattice-Boltzmann equation, dissipative particle dynamics, and stochastic rotation dynamics. One of the most commonly asked questions is how do the various methods compare in terms of accuracy and computational cost. At present there is no meaningful answer, in part because it is not straightforward to construct clean test calculations and obtain reference solutions to these problems. I will outline some principles that may be helpful in developing a basis for comparison and describe preliminary results obtained with the lattice-Boltzmann method.

1Research on aspects of the Paradigms in Physics Program is funded by the National Science Foundation under DUE 06-18877.

2This work was supported by the National Science Foundation (CTS-0505929)
12:15PM Q8.00006 Non-equilibrium Crystallization Kinetics of an Induced Transition Observed in a Nano-Colloidal Liquid Crystal-Aerosil Dispersions 1, DIPTI SHARMA, Worcester Polytechnic Institute — A new transition feature, termed “Induced Crystallization” (IC), has been observed in a nano-colloidal liquid crystal (octyloxybenzophenyl, 8CB) and aerosol gel system dependent on silica content. This IC feature exhibits apparent activated kinetics following Arrhenius-like behavior. Temperature scans were performed on heating using a DSC technique at ramp rates from 1 to 20 K/min and the aerosol density varied from 0 to 0.2 g/cc. For the 8CB-sil, a well resolved exothermic peak was found as an additional feature on heating scan before the melting transition, absent in bulk 8CB. As the sil density increases, the observed the enthalpy increases while the effective activation energy decreases for this IC feature, eventually saturating at the highest density studied. This behavior appears consistent with molecular disorder imposed by the surface molecular interaction, inducing slow glassy crystallization of the 8CB liquid crystal.

1Author is grateful to Germano Iannacchione for many useful discussions.

12:27PM Q8.00007 Phase separation in asymmetric 2D binary hard-sphere mixtures 1, CAMILO GUAQUETA, ERIK LÜJTEN, University of Illinois at Urbana-Champaign — We investigate the phase behavior and structural properties of highly asymmetric binary mixtures of additive hard spheres in two dimensions, using Monte Carlo simulations in both the canonical and restricted Gibbs ensembles. To tackle large diameter ratios between the large and small species we use an efficient geometric cluster algorithm. Results for the pair correlation functions, compressibility, and depletion potentials are presented and compared to theoretical predictions, for diameter ratios from $q = 2$ to $q = 400$ and over a wide range of packing fractions. We explore and comment on the possibility of a demixing transition at high $q$ and total packing fraction.

This work is supported by the National Science Foundation through Grant No. DMR-0346914.

12:39PM Q8.00008 Experiments on a two dimensional lattice of charged colloids above a water-oil interface, WILLIAM IRVINE, YAEL ROICHMANN, ANDREW HOLLINGSWORTH, DAVID GRIER, PAUL CHAIKIN, Department of Physics and Center for Soft Matter Research, New York University — Charged hydrophobic (PMMA) colloids in an oil phase (cyclohexyl bromide) are attracted, without wetting, by image charge effects to an oil-water interface. The micron size spheres form a monolayer on the interface and interact via screened coulomb interactions to form a crystalline or hexatic lattice, depending on the tunable ratio of lattice spacing to screening length. We study the statics and dynamics of this system in periodic, commensurate, incommensurate, random and quasi-periodic potentials applied by holographic optical tweezers. The use of holographic tweezers allows considerable control over the character and strength of the applied potential. A similar system has been used to study the effects of a curved fluid interface on the particle density and on topological defects.

12:51PM Q8.00009 Nematic Order on Foams, BRYAN CHEN, RANDALL KAMIEN, University of Pennsylvania — We investigate the competition between nematic order and area minimization in nematic foams, in particular, how the structure is affected by the bending of the nematic director, and whether these systems will continue to obey Plateau’s laws. We study the minimum energy configurations of the director field on a one parameter family of perturbed Reuleaux tetrahedra with special attention to the location of topological defects. We determine the energy distribution at the Plateau borders versus the film surface and relate the change in structure to changes in elastic constants and surface tension.

1:03PM Q8.00010 Restricted Defect Dynamics in Colloidal Peanut Crystals, SHARON GERBODE, Physics - Cornell University, STEPHANIE LEE, Materials Science and Engineering - Cornell University, BETTINA JOHN, Chemical Engineering - Cornell University, ANGIE WOLFGANG, Physics - Cornell University, CHEKESHA LIDDELL, Materials Science and Engineering - Cornell University, FERNANDO ESCOBEDO, Chemical Engineering - Cornell University, ITAI COHEN, Physics - Cornell University — We report that monolayers of hard peanut-shaped colloidal particles consisting of two connected spherical lobes order into a crystalline phase at high area fractions. In this “lobe-closed-packed” (LCP) crystal, the peanut particle lobes occupy triangular lattice sites, much like close-packed spheres, while the connections between lobe pairs are randomly oriented, uniformly populating the three crystalline directions of the underlying lattice. Using optical microscopy, we directly observe defect nucleation and dynamics in sheared LCP crystals. We find that many particle configurations form obstacles blocking dislocation glide. Consequently, in stark contrast to colloidal monolayers of close-packed spheres, single dislocation pair nucleation is not the only significant energetic barrier to relieving an imposed shear strain. Dislocation propagation beyond such obstacles can proceed only through additional mechanisms such as dislocation reactions. We discuss the implications of such restricted defect mobility for the plasticity of LCP crystals.

1:15PM Q8.00011 Two-dimensional Dimer System, XIAOCHAO XU, DAVID PINE, Dept. of Physics and CSMR, New York University — We report on an experimental study of the two-dimensional phase behavior of colloidal dumbbells (dimers) trapped at a water-air interface. The dimers are made out of 1.6 μm silica microspheres that are fused together at a point. The water-air interface is very slightly concave so that the dimers are gently compressed by gravity towards the center of interface. The spheres form a stable dense state after a few days. For this dense phase, the location of peaks of both positional and angular pair correlation functions of the dimers reveals that many different orientations and configurations of the dimers are present and this is in agreement with the disorder crystal phase predicted by Monte Carlo Simulation. We found that there is a relatively long range angular correlation, but the positional correlation is short-ranged. This long range angular correlation is limited by the domain sizes which are determined by the density of the defects in the system.


1:27PM Q8.00012 Observing liquid-gas nucleation in a colloid-polymer solution using digital holographic microscopy, RYAN MCGORTY, VINOTHAN N. MANOHARAN, Harvard University — We study liquid-gas nucleation in a colloid-polymer solution. Though the colloidal particles are too small to resolve, we are able to observe nucleating droplets due to the refractive index mismatch between the two fluid phases. By using digital holographic microscopy we are able to observe the three-dimensional structure of the nucleating phase. The experimental setup and algorithms for reconstructing the holography data will be discussed. We hope that our data will allow us to better understand nucleation kinetics and that analysis of the fluctuating droplets will provide us with the surface tension between the two phases.

1:39PM Q8.00013 Soft Spheres Make More Mesophases, CHRISTIAN SANTANGELO, Department of Physics, University of Massachusetts, Amherst MA 01003, MATTHEW GLASER, Department of Physics, University of Colorado, Boulder CO 80309-0390, USA, GREGORY GRASON, Department of Polymer Science, University of Massachusetts, Amherst MA 01003, USA, RANDALL KAMIEN, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia PA 19104, USA, ANDREJ KOSMRLJ, Massachusetts Institute of Technology, Cambridge, MA 02139-4307, USA, PRIMOZ ZIHERL, Department of Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia — We use both mean-field methods and numerical simulation to study the phase diagram of classical particles interacting with a hard-core and repulsive, soft shoulder. Despite the purely repulsive interaction, this system displays a remarkable array of aggregate phases arising from the competition between the hard-core and shoulder length scales. In the limit of large shoulder width to core size, we argue that this phase diagram has a number of universal features, and classify the set of repulsive shoulders that lead to aggregation at high density. Surprisingly, the phase sequence and aggregate size adjusts so as to keep almost constant inter-aggregate separation.
1:51PM Q8.00014 Correlations between Dynamical Heterogeneities and Visco-elastic properties of Confined Colloidal Thin Films, PRASAD SARANGAPANI, Y. ELAINE ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN 46556 — Our recent study on confined hard-sphere colloidal suspensions demonstrates that glass transition can be observed ‘sooner’ as film thickness approaches a critical value while volume fraction remains constant. In this talk, we present a new study of the rheological properties of strongly confined colloidal thin films by using a home-designed micro-rheometer interfaced with a confocal microscope. We visualize the shear-induced structural relaxation at a single particle level and measure the rheological properties of confined colloidal thin films between two surfaces at narrow gap spacing ranging from 50 μm to 1-2 μm. The application of shear excitation greatly accelerates structural relaxation compared to quiescent colloidal fluids and we visualize particle displacements during the “bond breakage” process in strongly confined thin films. Additionally, we characterize their patterns, size and lifetimes under varied shear rates, and correlate their behaviors to the measured visco-elastic and visco-plastic properties of confined colloidal thin films.

2:03PM Q8.00015 Direct Imaging of the Collapsed Langmuir Monolayers and Multilayer Formation, DOSEOK KIM, Department of physics and Interdisciplinary Program of Integrated Biotechnology, Sogang University, SANGJUN SEOK, Department of Physics, Sogang University, TAE JUNG KIM, YOUNG DONG KIM, Nano-Optical Property Laboratory and Department of Physics, Kyung Hee University, DAVID VAKNIN, Ames Laboratory, Iowa State University — In-situ ellipsometry imaging was used to monitor Langmuir monolayer of arachidic-acid spread on water and on CaCl2 solution before and after collapse. The Langmuir monolayer was collapsed by compressing it beyond the minimal closely-packed surface molecular area. The ellipsometry image showed clear domains of collapsed regions, and analysis of the image allowed determination of thicknesses of these domains. It was found that the structure of multilayer domains in the collapsed region was bilayer of arachidic acid on the surface of CaCl2 solution, while the trilayer was formed on the pure water surface.

Wednesday, March 12, 2008 11:15AM - 2:03PM — Session Q9 DFD: Focus Session: DNA and Biofluid Analysis with Micro and Nanofluidic Devices Morial Convention Center R07

11:15AM Q9.00001 Using hydrodynamics to control DNA conformation for genotyping, sorting, and analysis, SUSAN MULLER, Univ. of California, Berkeley — Understanding the dynamics of biopolymers in complex flows is critical for the successful design of lab-on-a-chip devices. Work by Chu, Shaqfeh, and others using both Brownian dynamics simulations and direct, single molecule visualization methods have yielded unprecedented insights into DNA dynamics in simple shear, planar extension, and a range of linear mixed flows. Here, we focus on two flows designed to stretch and manipulate DNA conformation for single molecule genotyping and analysis; that is, flows designed to produce specific conformation fields. First, we present results on DNA in pressure-driven flow through a post array, and discuss insights from direct comparisons with Brownian Dynamics simulations by Shaqfeh and co-workers. Second, we consider stagnation point flows and, through the use of sequence-specific probes, demonstrate the potential of these flows for target sequence identification, single molecule studies of enzyme kinetics, and sorting.

11:51AM Q9.00002 Droplet-based microfluidics for high-throughput scanning of a large probe library, ADAM ABATE, DAVE WEITZ, Harvard University — Droplet-based microfluidics can produce monodisperse picoliter size microreactors at 10 kHz speed. We use this technology to prepare and fuse two drop trains. The drops in one train each contain a unique biochemical probe. The drops in the other train contain a probe target, enzymes, and other biochemical reagents that are necessary to sufficiently mimic the cellular environment. We synchronize the trains hydrodynamically and use electro-coalescence to perform high-throughput controlled fusion of one of each type of droplet microreactor. Using a multicolor laser excitation and fluorescence polarization detector we monitor each fusion event to observe the state of the probe and extract information about the target. This allows us to scan through a large probe library in a matter of seconds using less than 1μL or reagent.

12:03PM Q9.00003 Distant-ion dragging of polarizable nanodroplets and solvated DNA on nanotubes, BOYANG WANG, PETR KRAL, University of Illinois at Chicago, PROF. KRAL’S RESEARCH GROUP TEAM — Long distance Coulombic coupling allows efficient molecular dragging at the nanoscale by moving electrons, ions and molecules [1]. We use molecular dynamics simulations to show that ions intercalated inside semiconducting single-wall carbon nanotubes (SWNT) can be solvated in polarizable nanodroplets adsorbed on the SWNTs, and the coupled systems can be dragged by electric fields [2]. We also demonstrated that solvated single-strand DNA molecules adsorbed on SWNTs can be driven by ionic solutions flowing inside the tubes. These phenomena could be applied in molecular delivery, separation, desalination and be integrated in modern lab-on-a-chip technologies. [1] Boyang Wang and Petr Kral, JACS 128, 15984 (2006). [2] Boyang Wang and Petr Kral, submitted.

12:15PM Q9.00004 Spontaneous and coherent Raman spectroscopy of microfluidic flows, RAJAN ARORA, GEORGI PETROV, VLADISLAV YAKOVLEV, University of Wisconsin-Milwaukee, UNIVERSITY OF WISCONSIN-MILWAUKEE TEAM — Identifying protein structure and understanding its conformational dynamics are the grand challenges for biomedical science. The advent and most recent progress of microfluidics holds a promise of successfully addressing the major issues of structure determination—protein crystallization—by greatly multiplexing the evaluated number of crystallization conditions and protein dynamics—protein folding—by achieving a microsecond scale mixing. The further success of these approaches will strangely depend on the availability of remote probes capable of non-invasive interrogating the structure of biological molecules. Vibrational spectroscopy offers superior structural and chemical sensitivity, which can be successfully applied for characterizing transitional kinetics in microfluidic channels. In particular Raman and CARS give the molecular fingerprint along with structural information that is not possible with conventional fluorescence measurements. Here we are investigating the potential applicability of spontaneous and coherent Raman spectroscopy for protein folding and crystallization. Under suitable experimental conditions coherent Raman is seen to be 100 times more efficient than conventional Raman.

12:27PM Q9.00005 Detection of Kinase Translocation Using Microfluidic Electropicative Flow Cytometry, CHANG LU, JUN WANG, NING BAO, LEELA PARIS, HSIIANG-YU WANG, ROBERT GEAHLLEN, Purdue University, West Lafayette, IN, BIOLOGICAL ENGINEERING COLLABORATION, PHARMACY COLLABORATION — Translocation of a protein between different subcellular compartments is a common event during signal transduction in living cells. Detection of these events has been largely carried out based on imaging of a low number of cells and subcellular fractionation/Western blotting. These conventional techniques either lack the high throughput desired for probing an entire cell population or provide only the average behaviors of cell populations without information from single cells. Here we demonstrate a new tool, referred to as microfluidic electropicative flow cytometry, to detect the translocation of an EGFP-tagged tyrosine kinase, Syk, to the plasma membrane in B cells at the level of the cell population. We combine electrophoresis with flow cytometry and observe the release of intracellular kinase out of the cells during electroporation. We found that the release of the kinase was strongly influenced by its subcellular localization. Cells stimulated through the antigen receptor have a fraction of the kinase at the plasma membrane and retain more kinase after electroporation than do cells without stimulation and translocation. This tool will have utility for kinase-related drug discovery and tumor diagnosis and staging.
12:39PM Q9.00006 DNA/Protein Concentration and Identification by Nano-Channel Electrokinet...
11:15AM Q10.00001 Vortex ratchets from asymmetric weak-pinning channels\(^1\), K. YU, T.W. HEITMANN, C. SONG, M.P. DEFEO, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — The dynamics of vortex flow in confined geometries can be explored with structured weak-pinning channels of superconducting a-NbGe surrounded by strong-pinning NbN channel edges. The lack of pinning allows the vortices to move through the channels with the dominant interaction determined by the shape of the channel walls. We have fabricated such weak-pinning channels with asymmetric sawtooth edges for controlling the motion of vortices. We present measurements of vortex dynamics in the channels and compare these with similar measurements on a set of channels with uniform width. While the uniform-width channels exhibit a symmetric response for both directions through the channel, the vortex motion through the asymmetric channels is considerably different, with substantial asymmetries in both the static depinning and dynamic flux flow. We report on the rich dependence on magnetic field and driving force amplitude for this vortex ratchet effect.

\(^1\)Supported by NSF DMR-0547147

11:27AM Q10.00002 Vortex dynamics in a single weak-pinning superconducting channel with a Corbino geometry\(^1\). T.W. HEITMANN, K. YU, C. SONG, M.P. DEFEO, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — We report transport measurements of vortex flow dynamics in nanofabricated weak-pinning channels of a-NbGe with strong-pinning NbN channel edges. The channels are arranged in circular patterns on a Corbino disk geometry with a radial bias current, thus eliminating the influence of edge barriers to vortex entry on the dynamics. We have developed a SQUID voltameter arrangement for resolving the flux flow voltage from a small number of vortices moving through such a single mesoscopic channel. We discuss the configuration of this measurement scheme, along with potential applications of this system for measuring the flow of vortices around single weak-pinning channels free from edge barriers.

\(^1\)Supported by NSF DMR-0547147

11:39AM Q10.00003 Spontaneous Transverse Voltage and Amplified Switching in Superconductors with Honeycomb Pinning Arrays, CYNTHIA OLSON REICHHARDT, CHARLES REICHHARDT, Theoretical Division, Los Alamos National Laboratory — Using numerical simulations, we show that a novel spontaneous transverse voltage can appear when a longitudinal drive is applied to type-II superconductors with honeycomb pinning arrays in a magnetic field near certain filling fractions. We find a coherent strongly amplified transverse switching effect when an additional transverse ac current is applied, even for very small ac current amplitudes. The transverse drive can also be used to control switching in the longitudinal voltage response. We discuss how these effects could be used to create new types of devices such as current effect transistors.

11:51AM Q10.00004 Anisotropic properties of superconducting niobium wire-networks, J. HUA, Z.L. XIAO, Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, A. IMRE, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, U. PATEL, Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, L.E. OCOLA, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, V. NOVOSAD, U. WELP, W.K. KWOK, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439 — By utilizing focused ion beam (FIB) patterning technique we were able to fabricate hole-arrays with interhole spacing down to 150 nm into superconducting niobium (Nb) films. This enabled us to have a large temperature range to explore the properties of Nb wire networks in which the superconducting strips between neighboring holes are comparable to the superconducting coherence length. We studied the anisotropy of these superconducting networks by measuring the critical temperatures and magnetoresistances at various magnetic field directions respect to the film surface. The effect of film thickness, hole diameter, interhole-spacing and the symmetry of the hole lattice on the anisotropy will be reported.

12:03PM Q10.00005 Vortex Matter in Magnet — Superconductor Hybrids, IGOR LYUKSYUTOV, TAMU — Arrays of magnetic nanowires in alumina template can create highly inhomogeneous and 1 g STA strong magnetic fields on the template surface. We discuss properties of vortex matter created by such magnetic nanostructures and an external field in thin superconducting film on the template surface. This includes possible phase diagrams, pinning properties and critical current. We predict possible types of hysteresis curves and I-V curves in such magnet-superconductor hybrid in a broad temperature range.

12:15PM Q10.00006 Comparing computer simulations to measurements of slow moving vortices in NbSe\(_2\). MICHAEL DREYER, JONGHEE LEE, HUI WANG, University of Maryland, BARRY BARKER, Lab. for Phys. Sci. — We observed slow moving vortices in NbSe\(_2\) using scanning tunneling microscopy (STM) at a temperature of 4.2 K driven by the slow decay of the magnetic field of our superconducting magnet. The velocity of the vortices depends on the rate of field decay (0.4 mT/day) and the distance of the STM tip from the center of the sample. In our case the velocities of the vortices are in the range of \(\mu\)m/s allowing for high spatially and (relatively speaking) temporal data series. In order to understand the details of the measurements we wrote a simple 2D simulation for moving vortices in a static potential landscape. The simulation allows for a variety of scenarios such as periodic/fixed boundaries, constant variable driving force, insertion/extraction of vortices, point/line defects in order to match the behavior of the velocity with time, showing periodic ‘spikes’, so far defied explanation. The results of the simulation as well as possible reasons for the velocity vs. time data will be discussed in detail.

12:27PM Q10.00007 Towards ordered flux flow in A15 superconductor V\(_3\)Si at high fields\(^1\). R. KHADKA, A.A. GAPUD, University of South Alabama, A.P. REYES, L. LUMATA, P.L. KUHNS, National High Magnetic Field Laboratory, D.K. CHRISTEN, Oak Ridge National Laboratory — The motion of flux quanta is observed in a high-quality superconducting single crystal of V\(_3\)Si with weak pinning and significantly reduced thermal fluctuations due to a critical temperature of less than 17 K. This opens up the possibility of approaching ordered, Bardeen-Stephen flux flow (BSFF). The flux flow resistivity \(\rho_{ff}\) associated with dissipative flux motion is observed in V-I curves as a high current transition to an ohmic curve whose dissipation level is below the normal-state level. Details of overcoming technical difficulties of using high currents are described. BSFF is expected to be manifested by a linear dependence of \(\rho_{ff}\) on applied field \(H\). Measuring from fields of 6 T up to 20 T, an approach to ohmic curves characteristic of BSFF are clearly distinguishable, along with other interesting features such as the “peak” effect in critical current \(J_c(H)\) seen only when the pinning energy density is comparable to the elasticity of the flux medium. This and further data and their interesting ramifications are discussed.

\(^1\)Research funded by University of South Alabama startup funds and Summer Professional Development Award.
12:39PM Q10.00008 Time-resolved infrared spectroscopy of superconducting NbTiN film near Hc1. JUNGSEKE HWANG, University of Florida, HAILONG ZHANG, University of Nebraska, DAVID H. REITZE, CHRISTOPHER J. STANTON, D. B. TANNER, University of Florida, G. LAWRENCE CARR, Brookhaven National Laboratory — We use subnanosecond time-resolved, pump-probe infrared spectroscopy to study vortex dynamics of a conventional superconductor, Nb0.5Ti0.5N near Hc1. The measurements were performed at the National Synchrotron Light Source, Brookhaven National Laboratory; Picosecond pulses from a near-infrared Ti:Sapphire laser were used as a pump and, subnanosecond pulses of infrared synchrotron radiation as a probe. We report detailed magnetic field dependences of the amplitude of photoinduced quasi-particles and the effective lifetime of the quasiparticles and also discuss vortex dynamics in the system near Hc1. Near Hc1, we observe an interesting deviation from the field-independent behavior of the effective lifetime at lower fields.

The research has been supported by the DOE through grant DE-FG02-02ER45984 at Florida and contract DE-AC02-98CH10886 at BNL.

12:51PM Q10.00009 Imaging the dynamics of single vortices on grain boundaries in YBa2Cu3Oy+δ thin films. B. KALISKY, B. NOWADNICK, Geballe Laboratory for Advanced Materials, Stanford University, S. WENDERICH, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, E. ZELDOV, Department of Condensed Matter Physics, Weizmann Institute of Science, J. KIRTLEY, IBM Research Division, Yorktown Heights, A. ARIANDO, H. HILGENKAMP, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, K. A. MOLER, Geballe Laboratory for Advanced Materials, Stanford University — We use a scanning Hall probe microscope with single vortex resolution to study the dynamics of single vortices on grain boundaries in YBa2Cu3Oy+δ thin films with 10 kHz bandwidth. In the presence of an applied current, we observe individual vortices hopping between pinning sites. Detecting the motion of individual vortices allows us to probe the very- low-voltage regime of the current -voltage (I - V) characteristic, at voltage levels of 2 . 10^-15 V. By scanning the grain boundary we show local I – V curves and investigate the statistical processes at the onset of vortex motion.

1:03PM Q10.00010 Imaging the Vortex Density of States in Bi2Sr2CaCu2O8+x. YI YIN, M. ZECH, T. L. WILLIAMS, Harvard University, GENDA GU, Brookhaven National Laboratory, J. E. HOFFMAN, Harvard University — We use a low temperature scanning tunneling microscope (STM) to image vortices in the high temperature superconductor Bi2Sr2CaCu2O8+x, in magnetic fields up to 9T. We locate the vortices via their increased local density of states near ±7 mV. We investigate the dependence of the vortex halo on several parameters, including applied magnetic field and proximity to surface impurities.

This work was supported by the Air Force Office of Scientific Research under grant FA9550-05-1-0371, and by the NSF under grant DMR-0508812.

1:15PM Q10.00011 Single Vortex Imaging and Shaking in a YBa2Cu3O6.991 Single Crystal. LAN LUAN, O. M. AUSLAENDER, Stanford University, E. ZELDOV, Weizmann Institute of Science, K. A. MOLER, Stanford University, D. A. BOÑN, RUIXING LIANG, W. N. HARDY, Department of British Columbia — We image and manipulate individual vortices in a detwinned YBa2Cu3O6.991 single crystal, using magnetic force microscopy (MFM). We observe a strong dynamic asymmetry between the fast and slow directions of the raster imaging pattern, when the MFM tip-vortex force exceeds the depinning force. The vortex can be dislodged hundreds of nanometers along the raster direction, while perpendicular to it, along the slow direction, it can be stretched up to several microns by the same applied force. We attribute this effect to single vortex shaking, in analogy with vortex matter shaking induced by an oscillating magnetic field or current. Here, we raster the tip, shaking the top of one vortex to help it explore different configurations, which are determined by the interplay between pinning and elasticity. In this process, elastic energy associated with stretching along the slow direction can be released, thus allowing the vortex to be dragged further. We are currently studying shaking in an underdoped YBa2Cu3O7-δ single crystal, where the Josephson coupling along crystal c-axis is much reduced, rendering elasticity weaker.

1:27PM Q10.00012 Tunneling of an extended object in a dissipative environment: suppression of tunneling of vortices caused by a remote gate. KAREN MICHAELI, Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, ALEXANDER FINKEL’STEIN, Weizmann Institute of Science, Israel and Department of Physics, Texas A&M University, USA. A strong decrease of the resistance of a superconducting film measured in magnetic field has been observed when a metallic gate is placed above the film. We study how the magnetic coupling between vortices in a superconducting film and electrons in a remote unbiased gate affects the tunneling rate of the vortices. We examine two approaches to analyze tunneling in the presence of low-energy degrees of freedom: (i) the response of the electrons inside the metallic gate to a change in the vortex position is described as “tunneling with dissipation” (ii) the scattering of the electrons by the magnetic flux of the vortex leads to the Orthogonality Catastrophe that opposes the vortex tunneling. We show that the gate can cause a dramatic suppression of the vortex tunneling restoring the superconducting property in accord with the experiment.

1:39PM Q10.00013 Dynamics of vortices driven by magnetic field changes observed by LT-STM. JONGHEE LEE, MICHAEL DREYER, HUI WANG, University of Maryland, BARRY BARKER, Lab. for Phys. Sci. — When changing the magnetic field for a type two superconductor the vortex density has to change accordingly. Vortices have to enter/leave the superconductor to facilitate that change. Since vortex-defect interactions impede the vortex motion such a change does not happen instantaneously. Observing the vortex lattice at a given distance from the center by STM allows to study that behavior. The velocity usually decays close to exponentially. Although the first ‘fast’ phase (30 min) is unaccessible to STM due to its limited scan speed the tail section (˜5 h) can be studied in detail. We will present analysis of the data and compare it to previous results on slow moving vortices driven by a slowly decaying magnetic field.

1:51PM Q10.00014 h/e-Flux Periodicity in Superconducting Loops. ARNO KAMPF, FLORIAN LOBER, THILO KOPP, JOCHEN MANNHART, CHRISTOF SCHNEIDER, University of Augsburg, YURI BARASH, Russian Academy of Sciences, Chernogolovka — We apply the BCS theory to superconducting rings with unconventional order parameter symmetries. An external magnetic flux changes the character of the states in the condensate; as a consequence the energy of the superconducting ground state varies with a flux period of h/e. This h/e periodicity is caused by the flux-induced reconstruction of the supercurrent carrying condensate.

Supported by the Deutsche Forschungsgemeinschaft through SFB 484.

Wednesday, March 12, 2008 11:15AM - 1:39PM —
Session Q11 DMP: Focus Session: Hybrid Magnetic-Superconducting Systems II
Morial Convention Center R09
Curie's intriguing finding was the reduction in the $S$ ordering temperature of the SRO layer when $T$ regions, arranged along narrow strips, where a superconductor-like gap penetrates the SRO more than 25 nm. This is attributed to "crossed Andreev reflections" bilayers indeed show that on most of the junction area the $S$ order parameter vanishes in the SRO over a distance less than 8 nm. However, we find localized a superconductor-ferromagnet ($S$-$F$) junction is spin polarized, Andreev reflections are suppressed. Consequently, the induced $S$ order parameter in the $F$ is $\Delta_{0}$ enhancement in cuprate bilayers. We have also studied (110)YBCO-SRO bilayers, where, surprisingly, a clear penetration of the Andreev bound states (residing on the (110) YBCO surface) into the $F$ layer was revealed. The penetration is manifested in the density of states as a split zero bias conductance peak with an imbalance between peak heights. Our data indicate that the splitting occurs at the $S$ side, possibly as a consequence of induced magnetization, consistent with recent theoretical predictions. The imbalance is attributed to the spin polarization in SRO.


Superconductor-Ferromagnet Bilayers

Scanning Tunneling Spectroscopy Study of Bi-Layer

La$_{0.7}$Ca$_{0.3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-\delta}$ Thin Films

I. FRIDMAN, P. MORALES, J.Y.T. WEI, University of Toronto — Recent experiments have reported long-range proximity effect in ferromagnet/superconductor (F/S) heterostructures comprised of transition-metal perovskites. To look for direct evidence of this effect, we have performed scanning tunneling spectroscopy (STS) on La$_{0.7}$Ca$_{0.3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-\delta}$ (LCMO/YBCO) bi-layer thin films. The bilayer films were epitaxially grown on SrTiO$_3$ substrates using pulsed laser deposition. STS measurements were made at 4.2 K on bi-layer films with varying LCMO thickness (20 to 60 nm) and in a magnetic field parallel to the film. The STS data were analyzed for spectral signatures of a pairing gap on the LCMO layer induced by the YBCO layer, to determine the length scale of the F/S proximity effect and the role played by magnetic domain walls.

Work supported by NSERC, CFI/OIT and the Canadian Institute for Advanced Research.

Anomalous Sub-Gap features in Nb/Ni Tunneling DOS

PAUL SANGIORGIO, MALCOLM BEASLEY, Stanford University, JUNHYUNG KWON, KOOKRIN CHAR, Seoul National University — We report the existence of anomalous sub-gap features in tunneling DOS measurements of Superconductor/Strong Ferromagnet bilayers. By measuring the DOS as a function of ferromagnet thickness, $d_F$, we are able to document the spatial evolution of the Cooper pairs diffusing into the ferromagnet. This technique proves to be much less sensitive to variations in boundary conditions and provides more detailed information per sample than traditional $T_e$ or $J_c$ measurements. In addition to the sub-gap features, we find that the DOS shows the usual peaks at $\pm \Delta_0$, which "invert" at $d_F = 3.5$ nm. We analyze the results with the fully non-linear Usadel equation, including the effects of various scattering mechanisms and spin-dependent boundary conditions. We are able to quantitatively account for the features at $\pm \Delta_0$ through the addition of spin-orbit scattering in the F-layer, but we find that no known parameter recreates the sub-gap features. By examining the behavior of the sub-gap in magnetic field, we propose that it is a signature of a long-range triplet condensate.

Spin Polarization And Inelastic Scattering In High And Low Transparency Ferromagnet/Superconductor Point Contacts

PAUL J. DOLAN, JR., Northeastern Illinois University, CHARLES W. SMITH, University of Maine — For point contact spectroscopy studies of ferromagnet/superconductor charge transport, the effects of spin polarization and inelastic scattering can dominate conductance data. Model calculations show that accurate values of the spin polarization parameter can most easily be determined in high transparency contacts (the ballistic limit) when inelastic scattering is low, and in low transparency contacts (the tunneling limit) when inelastic scattering is high. Comparison with data for both contacts will be shown.

Electrical properties of interfaces in high-$T_c$ superconducting heterostructures

MAARTEN VAN ZALK, JOS BOSCHKER, MENNO VELDORST, ALEXANDER BRINKMAN, HANS HILGENKAMP, Condensed Matter Physics and Devices Group, MESA+ Institute for Nanotechnology, University of Twente — Electrical contacts between materials of different functionality are often required, both for technological applications as well as for fundamental research. However, contacts between different complex oxides frequently do not behave like expected. For example, it is well known that tunnel junctions are difficult to fabricate from high-$T_c$ superconductors, due to the presence of a degraded, non-superconducting layer underneath the tunnel barrier. We investigated the interface properties of a number of different oxide heterostructures, prepared by pulsed laser deposition. Specifically, the causes of non-ideal interface behavior, such as changes in the stoichiometry, oxygen deficiency, structural changes and electronic reconstruction, were investigated.

All-oxide inverse superconducting spin switch

JACOBO SANTAMARIA, GFMC, Fisica Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain, NORBERT NEMES, ICMC-CSIC, 28049 Cantoblanco, Spain, CRISTINA VISANI, JAVIER GARCIA-BARRIOCANAL, ZOUHAIR SEFRIOU, DIEGO ARIAS, CARLOS LEON, GFMC, Fis. Aplicada III, Univ. Complutense Madrid, Spain, MAR GARCIA-HERNANDEZ, ICMC-CSIC, Cantoblanco, Spain, SUZANNE TE VELTHUIS, AXEL HOFFMANN, Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — In proximity coupled ferromagnet/superconductor/ferromagnet (F/S/F) structures the critical temperature is modulated by the relative orientation of the magnetization in the F layers (superconducting spin switch-SSS). A larger $T_{c}$, with antiparallel (AP) compared to parallel (P) magnetizations results from the averaging of the exchange field over the coherent volume. Recent reports have shown an SSS behavior in F/S/F structures with strong ferromagnets, where superconductivity is favored for $P$ orientation of the adjacent magnetizations. Its origin is a subject of debate. While some reports suggest enhanced pair breaking by spin-polarized quasiparticles in the AP configurations, others emphasize the effect of stray fields in depressing the superconductivity. Comparing data of bilayers and trilayers, we show that the SSS effect of our epitaxial LCMO/YBCO/LCMO structures is governed by spin transport within the F layers.

Covalent Bonding and Orbital Reconstruction at an Oxide Interface.

JAK CHAKHALIAN, University of Arkansas, JOHN FREELAND, Advanced Photon Source, Argonne National Laboratory, HANS-ULRICH HABERMEIER, GEORG CRISTIANI, G. KHALIULLIN, Max Planck Institute for Solid State Research, MICHEL VAN VEENENDAAL, Northern Illinois University, BERNHARD KEIMER, Max Planck Institute for Solid State Research — Atomically controlled interfaces between two materials can give rise to novel physical phenomena and functionalities. Modern synthesis methods have yielded high-quality heterostructures of oxide materials with competing order parameters. Orbital reconstructions and covalent bonding must be considered as important factors in the rational design of oxide heterostructures. Here we examine the interface between high-temperature superconducting (Y,Ca)Ba$_2$Cu$_3$O$_{7+\delta}$ and metallic La$_2$Cu$_3$O$_6$ by resonant x-ray spectroscopy. The resulting data show that electrons are transferred from Mn to Cu ions across the interface. This phenomenon is accompanied by the major reconstruction of the orbital occupation and symmetry in the CuO$_2$ plane. Specifically, we report the experimental finding that unlike bulk at the interface Cu d$_{3z^2-r^2}$ orbital is partially occupied and electronically active. This observation opens a path to orbital engineering of interface-controlled materials. J. Chakhalian et al, "Covalent Bonding and Orbital Reconstruction at an Oxide Interface," Science, v. 318, 1155 (2007).
observed in the resistivity data, the lower two transitions are suppressed by an applied magnetic field. At low temperatures metamagnetism is observed in the and high magnetic field measurements of the electrical resistivity and magnetization. For zero field, three magnetic transitions at 1 K, 1.5 K and 2.8 K are reveal that the superconductivity coexists with the hidden order but is suppressed by antiferromagnetic ordering. Here, we report charge and thermal transport by itself is an exceptional case of pairing among heavy electrons with a long Fermi-wavelength in a nearly semimetallic system. Moreover, pressure studies conductivity with such a low density is remarkable since the superfluid density is very low in some way reminiscent of underdoped cuprates; the superconductivity observations, most of the carriers disappear below \( T_\alpha \) alignment is changed from parallel to antiparallel in FSF. Moreover, the critical Josephson current in SFFS multilayers is also a monotonic function of \( \alpha \) when the junction is far enough from \( 0-\pi \) transitions. In contrast to the diffusive case, no substantial impact of long-range spin–triplet superconducting correlations neither on conductance nor on the Josephson current has been found in the clean limit.

1:15PM Q11.00009 Properties of Hybrid Superconductor/Half-metal Systems, MATTHIAS ESCHRIG, University of Karlsruhe and DFG-Center for Functional Nanostructures, D-76128 Karlsruhe, Germany, TOMAS LOFWANDER, Chalmers University of Technology, S-412 96 Gothenburg, Sweden — Interfaces between materials that exhibit different types of order present unique opportunities to study fundamental problems in physics. One example is the interface between a single superconductor and a half-metallic ferromagnet, where Cooper pairing occurs between electrons with opposite spin on one side, while the other displays 100% spin polarisation. New effects, like spin mixing and spin rotation are characteristic for such interfaces [1], providing a mechanism for conversion between unpolarized and completely spin polarized supercurrents. Our predictions have been confirmed in a recent experiment observing a supercurrent through half-metallic CrO\(_2\) [2]. The interface region exhibits a superconducting state of mixed-spin pairs with highly unusual symmetry properties that opens up new perspectives for exotic Josephson devices [3]. We present results for Andreev bound state spectra for point contact Andreev conductance spectra. The role of disorder and symmetry of the pairing amplitudes on the spectra and the temperature dependence of the Josephson current is elucidated.

1:27PM Q11.00010 Novel Josephson junctions of high-\( T_c \) cuprate using magnetic islands: Fabrication and Properties, A. MAEDA, L. GOMEZ, S. KITAMURA, Department of Basic Sciences, University of Tokyo — In spite of the potential high performance, no one has succeeded in fabricating good Joseph junctions of high-\( T_c \) cuprate superconductors with a large \( I_c R_N \) product and textbook like \( I_c - V \) characteristics. This is probably because the fabrications of the oxide barrier layer even on the almost perfect surface of the cuprate causes many unexpected troubles, suggesting that there are still many issues to be solved in the surface science of the cuprate superconductors. We have tried the high-\( T_c \) Junction fabrication with a novel method, where we do not need to fabricate oxide barrier layer; A small island of Fe was merely placed on a strip of a cuprate superconductor, LSCO. By measuring \( I_c - V \) characteristics, microwave radiation effect, and magnetic field effect, it turned out that this simple novel structure becomes a typical Josephson junction. What is remarkable is that the structure often exhibits a large \( I_c R_N \) value (\( \sim 10-20 \) meV), suggesting that our method is promising. Together with various kinds of comparative experiments, we will discuss the mechanism of the weak coupling.

Wednesday, March 12, 2008 11:15AM - 2:03PM
Session Q12 DCMP: Focus Session: Hidden Order and Heavy Fermions Morial Convention Center 203

11:15AM Q12.00001 Exotic Superconducting State Embedded in the Hidden Order Phase of URu\(_2\)Si\(_2\)\(^1\), YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan — The heavy-Fermion compound URu\(_2\)Si\(_2\) has mystified researchers since the superconducting state \( (T_c = 1.5\) K) is embedded within the “hidden order” phase \( (T_h = 17.5\) K). According to several experimental observations, most of the carriers disappear below \( T_h \), resulting in a density one order of magnitude smaller than in other heavy-Fermion superconductors. Superconductivity with such a low density is remarkable since the superfluid density is very low in some way reminiscent of underdoped cuprates; the superconductivity by itself is an exceptional case of pairing among heavy electrons with a long Fermi-wavelength in a nearly semimetallic system. Moreover, pressure studies reveal that the superconductivity coexists with the hidden order but is suppressed by antiferromagnetic ordering. Here, we report charge and thermal transport measurements on ultraclean single crystals of URu\(_2\)Si\(_2\) \( (RRR < 700) \) down to 30 mK \( (T_c/50) \), which reveal a number of unprecedented superconducting properties. The uniqueness is best highlighted by field-induced superconductor-insulator-like first-order transition at the upper critical fields, which is a direct consequence of the electronic structure imposed by the hidden order. The results provide strong evidence for a new type of unconventional superconductivity with two distinct gaps having different nodal topology. We propose a gap function with chiral \( d \)-wave form \( \Delta_k \propto k_c (\pm i k_y) \) [1]. We also report a distinct flux line melting transition with outstanding characters and a formation of the quasiparticle Bloch state in the periodic flux line lattice in this ultraclean system [2]. The intriguing superconducting state of URu\(_2\)Si\(_2\) adds a unique and exciting example to the list of unconventional superconductors.

1:27PM Q11.00008 Spin-triplet correlations in clean superconductor-ferromagnet multilayers, MATTHIAS ESCHRIG, MATTHIAS ESCHRIG, ZORAN RADOVIC, ZORICA PAJOVIC, MILOS BOZOVIĆ, Department of Physics, University of Belgrade, POB 368, 11001 Belgrade, Serbia, JEROME CAYSSOL, ALEXANDER BUZDIN, Univeristie Bordeaux I, CPMOH, UMR 5798, 33405 Talence, France — We study transport phenomena in clean superconductor-ferromagnet (S-F) multilayers for a general case of arbitrary relative orientation of in-plane magnetizations and interface transparencies. The scattering problem based on the Bogoliubov-de Gennes equation is solved, taking into account both spin-singlet and spin-triplet superconducting correlations in two geometries, FSF and SFFS. We find a monotonic dependence of conductance spectra on the angle of misorientation of magnetizations \( \alpha \) as their alignment is changed from parallel to antiparallel in FSF. Moreover, the critical Josephson current in SFFS multilayers is also a monotonic function of \( \alpha \) when the junction is far enough from \( 0-\pi \) transitions. In contrast to the diffusive case, no substantial impact of long-range spin–triplet superconducting correlations neither on conductance nor on the Josephson current has been found in the clean limit.

11:51AM Q12.00002 Neutron scattering studies of the quantum critical point of CeAuSb\(_2\), JOHN JANIK, CHRIS WEBE, NHMFL/FSU, HAIDONG ZHOU, NHMFL, BEN UELAND, YING CHEN, JEFF LYNN, NIST, ZACHARY FISK, University of California, Irvine, H. LE, WEI BAO, LANL, YOUN-JUNG JO, LUIS BALICAS, NHMFL — We present neutron scattering results on CeAuSb\(_2\), a quantum critical material whose critical point in revealed in magnetic field. We find incommensurate ordering, indicative of itinerant electron physics. The incommensurate feature seem to be directly related to metamagnetic transitions.

12:03PM Q12.00003 Magnetic and electrical transport study of single crystal Yb\(_2\)Au\(_3\), H. RYU, E.D. MUN, S.L. BUDKO, P.C. CANFIELD, Ames Lab / Iowa State University — Single crystals of Yb\(_2\)Au\(_3\) grown by flux method are studied by low temperature and high magnetic field measurements of the electrical resistivity and magnetization. For zero field, three magnetic transitions at 1 K, 1.5 K and 2.6 K are observed in the resistivity data, the lower two transitions are suppressed by an applied magnetic field. At low temperatures magnetism is observed in the magnetization and magnetoresistance data. Strong anisotropy between the tetragonal ab plane and c-axis, is revealed in both magnetization and transport measurements. The \( H - T \) phase diagram for applied field along the \( ab \) plane is constructed by electrical transport measurements. The anisotropy can be explained with a crystalline electric field (CEF) model. Yb\(_2\)Au\(_3\) can be characterized as Kondo lattice compound with strong CEF splitting.


\(^2\)Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.
12:15PM Q12.00004 A Novel Low-Temperature Phase in Strongly Correlated CePd$_3$Ga$_2$. QINC'AN LI, J.F. MITCHELL, K.E. GRAY, Argonne National Laboratory, ROBIN MACALUSO, Northern Colorado College — The specific heat, $C_p$, of CePd$_3$Ga$_2$ strongly supports the presence of two phase transitions, which are consistent with magnetization data. The 11 K transition (suppressed for fields, $B>3$ T) is also seen in the resistivity, whereas the 6 K transition is not. The resistivity is anisotropic both with respect to field and current directions, while its temperature dependence is similar to UCd$_3$ and CeAuSb$_2$. Both resistivity and $C_p$ are affected by magnetic fields up to about 30 K and possible connections will be discussed.

1Supported by US DOE, BES under contract DE-AC02-06CH11357.

12:27PM Q12.00025 Is the Low-Temperature Phase in CePd$_3$Ga$_2$ Fascinating or Just Novel? K.E. GRAY, J.F. MITCHELL, H. CLAUS, QINC'AN LI, Argonne National Laboratory, ROBIN MACALUSO, Northern Colorado College — Magnetization data for CePd$_3$Ga$_2$ strongly support the presence of two phase transitions, also seen in specific heat, $C_p$. The 11 K transition (suppressed for fields, $B>3$ T) has similarities to UCd$_3$ and CeAuSb$_2$, but the lower temperature phase ($T<6$ K, $B<2.5$ T) is novel and its nature is a mystery. Its uniaxial magnetic anisotropy implies that CePd$_3$Ga$_2$ is an effective Ising system for the Ce spins, likewise consistent with $C_p$. The phase diagram of this fascinating material will be discussed in terms of combined magnetization, conductivity, $C_p$ and neutron scattering data.

1Supported by US DOE, BES under contract DE-AC02-06CH11357.

12:39PM Q12.00006 Field-induced magnetic phase transition in antiferromagnetic YbPtSi$^1$. YURI JANSSEN, Brookhaven National Laboratory, YUEN YIU, Stony Brook University, PETER KHALIFA, MEIGAN ARONSON, Brookhaven National Laboratory, Stony Brook University, Berkeley National Laboratory, State University of New York at Stony Brook. — We have studied single crystals of the orthorhombic intermetallic compound YbPtSi. Here we present results of anisotropic field- and temperature dependent magnetization and specific heat. Magnetization isotherms measured between 1.8 K and the ordering temperature of 4.65 K show a sudden anomalous increase in magnetization. This phase transition becomes sharper and takes place at progressively higher fields as temperature decreases. Measurements of field- and temperature dependent specific heat above 0.4 K confirm this magnetic phase transition above 1.8 K, and allow us to draw anisotropic magnetic phase diagrams down to 0.4 K. These phase diagrams indicate that the magnetic phase transition in YbPtSi can be brought close to zero temperature in relatively modest applied fields, $\sim 3.5$ T for the hard magnetization direction. The critical line is well described by $Y_e/(H/T)^{1/2} = (1-(H_e(T)/H_e(0))^{2})^{0.3}$, very different from quasi-one-dimensional or two-dimensional quantum critical antiferromagnets.

$^1$This research is supported by US-DOE, under contract DE-AC02-98CH10886.

12:51PM Q12.00007 Magnetic Order in single-crystalline YbPtSi. YUEN YIU, State University of New York at Stony Brook, YURI JANSSEN, Brookhaven National Laboratory, PETER KHALIFA, MEIGAN ARONSON, Brookhaven National Laboratory, State University of New York at Stony Brook. MOOSUNG KIM, Brookhaven National Laboratory, MARCUS BENNETT, State University of New York at Stony Brook. — We report the first measurements on YbPtSi, which we synthesized as single crystals by means of flux growth from Indium. Single crystal x-ray diffraction measurements find that the YbPtSi crystal structure is the orthorhombic C$_2$Si$_2$-type, with one crystallographic site for Yb. Magnetic susceptibility measurements find Curie-Weiss behavior above 100 K with a moment of $3.45 \mu_B$, close to the 4.54 $\mu_B$ expected for trivalent Yb. Measurements of the heat capacity find a mean field-like magnetic ordering transition at $T=4.65K$. DC-susceptibility measurements show substantial single ion anisotropy, but also exhibit a peak at 4.65 K, indicating possible antiferromagnetic ordering. The electrical resistivity is metallic, and the magnetic ordering is accompanied by a change in slope. The magnetic entropy amounts to only about 65% of $Rln2$ expected from an ordering state doublet at the ordering temperature, suggesting a possible role for the Kondo effect. Our measurements indicate that YbPtSi is an unusual example of an Yb-based Kondo lattice system, ordering at an unusually high temperature.

1:03PM Q12.00008 Angle resolved photoemission studies of YbRh$_2$$_{1-x}$Ge$_x$_2. S.-K. MO, K. TANAKA, N. MANNELLA, Stanford University and Advanced Light Source, C. CAPAN, D.J. KIM, Z. FISK, UC Irvine, Z. HUSSAIN, Advanced Light Source, Z.-X. SHEN, Stanford University, YUEN YIU, Brookhaven National Laboratory. — YbRh$_2$_2 is a prototype system for 4f-based Kondo lattices and has attracted a lot of attention as the first Yb-based system with a quantum critical point (QCP) at $x \sim 0.05$. The QCP can be tuned by either magnetic field or chemical substitution, and non Fermi liquid properties have been observed in the vicinity of it. We present high-resolution angle resolved photoemission data on this compound as a function of Ge-doping. The result will be discussed in conjunction with various theoretical proposals on the Fermi surface topology of this material.

1:15PM Q12.00004 High Pressure Studies of CeIn$_3$ in High Magnetic Fields. JACOBY COOLEY, Los Alamos National Laboratory, RONGWEI HU, Brown University, ROSS MCDONALD, National High Magnetic Field Laboratory - LANL, CEDOMIR PETROVIC, Brookhaven National Laboratory, STANLEY TOZER, National High Magnetic Field Laboratory - FSU. — High pressure and strong magnetic fields are useful tools for studying the relationship between the antiferromagnetism and unconventional superconductivity observed in the heavy fermion superconductor CeIn$_3$. We report high pulsed magnetic field (up to 55 T) pressure studies of single crystal CeIn$_3$ utilizing the change in the resonant frequency of a tunnel diode oscillator (TDO) as a contactless means of measuring the skin depth of the crystal. An anomaly in the skin depth was observed at $\sim 42$ T and was found to be driven to lower fields with increasing pressure. The relationship of the observed anomaly with the nature of the Fermi surface and the formation of a superconducting state at $\sim 200$ mK and 27 kbar will be discussed. 1. N. Harrison et al, preprint arXiv:07062387 2. N. D. Mathur et al, Nature, 394, 39 (1998)
1:39PM Q12.00011 Unconventional Magnetic Scaling Exponents near a $T = 0$ Transition in URu$_2-x$Re$_x$Si$_2$\textsuperscript{1}, NICHOLAS P. BUTCH, BENJAMIN T. YUKICH, M. BRIAN MAPLE, Department of Physics and Institute for Pure and Applied Physical Sciences, University of California, San Diego — Substituting Re for Ru in the heavy fermion compound URu$_2$Si$_2$ suppresses the hidden order and superconducting transitions and gives rise to long range ferromagnetism. From electrical transport, specific heat, and magnetic susceptibility studies of single crystals of URu$_2-x$Re$_x$Si$_2$, $0 \leq x \leq 0.6$, it is apparent that the non-Fermi liquid behavior first observed in polycrystalline samples is indeed a robust phenomenon intrinsic to the bulk material. We present a recent investigation of the magnetization of URu$_2$Si$_2$ and find the magnetic transition from well into the ferromagnetic phase down to its onset. The variation of the exponents with $x$ is discussed within the context of the observed non-Fermi liquid behavior.

\textsuperscript{1}This research was supported by the US National Science Foundation and US Department of Energy.

1:51PM Q12.00012 The linear and non-linear magnetic susceptibility of URu$_2$Si$_2$ in hydrostatic pressure, G.J. MACDOUGALL, G.M. LUKE, McMaster University, T. GOKO, TRIUMF, J.D. GARRETT, McMaster University — The heavy-fermion material URu$_2$Si$_2$ has long been a topic of interest due to the mysterious 'hidden order' transition at $T_0=17.5K$. Though the exact nature of this order is still a matter of great debate, the transition has strong signatures in heat capacity, resistivity and linear and non-linear magnetic susceptibility. Interest in the material has increased in recent years, as high-pressure measurements have revealed a first-order quantum phase transition to an antiferromagnetically ordered state. However, the fate of the hidden-order, and how it relates to the anti-ferromagnetism is still unknown. With this in mind, we have measured the linear and nonlinear magnetic susceptibility of single-crystalline URu$_2$Si$_2$ under hydrostatic pressure. We will report the results of these measurements, with particular emphasis placed on the signatures of hidden-order and how they evolve as the system is driven into the antiferromagnetic state.

Wednesday, March 12, 2008 11:15AM - 1:51PM —
Session Q13 DCOMP: Ground State Density Functional Theory: Applications

11:15AM Q13.00001 Polarizabilities and Hyperpolarizabilities of Hydrogen Chains: Is Self-Interaction Correction the Key?, A. RUZINSZSKY, J.P. PERDEW, Dept. of Physics, Tulane U., G.I. CSONKA, Dept. of Chemistry, Budapest U. of Technology and Economics, G.E. SCUSERIA, Dept. of Chemistry, Rice U., O.A. VYDROV, Dept. of Chemistry, MIT — Semi-local density functionals like the local spin density and generalized gradient approximations are known to overestimate [1, 2] the polarizabilities and especially the hyperpolarizabilities of long-chain molecules, while these quantities are much better predicted by exact-exchange methods (Hartree-Fock or Optimized Effective Potential). The source of this failure of the semilocal approximations for the electric response is rooted in the self-interaction error inherent to the semilocal approximations. We show here that the semilocal functionals, after full or scaled-down Perdew-Zunger self-interaction correction [3, 4], are even better than the exact-exchange methods for these quantities.


11:27AM Q13.00002 Improved Description of Stereoelectronic Effects Using Semi-local Density Functional Theory, GABOR I. CSONKA, Dept. of Chemistry, Budapest U. of Technology and Economics, Budapest, Hungary, JOHN P. PERDEW, ADRIENN RUZINSZKY, Dept. of Physics, Tulane U., New Orleans LA 70118 — Proper description of stereoelectronic (SE) effects is desirable for any theoretical method to be used in organic chemistry. The SE design rules are frequently used in synthetic organic chemistry to design and explain new reactions by electron donating and withdrawing effects or steric interactions. These effects are often poorly described by standard generalized gradient approximations for exchange and correlation. Many popular exchange-correlation functionals are biased toward the correct description of free atoms and fail to improve upon LSDA for solids. Changing two parameters within the PBE form to satisfy different constraints leads to a new non-empirical GGA, PBEsol [1], that performs well for solids and improves the description of large organic systems and reactions. We present examples where this new non-empirical functional provides considerable improvements for molecules. [1] J.P. Perdew, A. Ruzinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, and K. Burke, http://arxiv.org/abs/0711.0156

11:39AM Q13.00003 Approximations in local hybrid density functionals, BENJAMIN JANESKO, Rice University, GUSTAVO SCUSERIA, Rice University — Hybrid density functionals incorporating a fraction of exact (Hartree-Fock-type) electronic exchange have become one of the dominant approximations for modeling the electronic structure of large molecules and solids. Generalization to a position dependent admixture of exact exchange provides a route to improved accuracy. However, such local hybrid functionals generally have a significant computational expense. We present work towards approximating density functionals that incorporate some of the desirable properties of local hybrids, without requiring explicit evaluation of exact exchange. These results show promise for extending the benefits of hybrid functionals to larger systems.

11:51AM Q13.00004 The role of middle-range Hartree-Fock-type exchange in hybrid functionals, THOMAS HENDERSON, ARTUR IMAYLOV, GUSTAVO SCUSERIA, Rice University, ANDREAS SAVIN, Universite Pierre et Marie Curie — While hybrid functionals are responsible for many successes in modern Kohn-Sham theory, they have several drawbacks. The slow decay of nonlocal exchange makes hybrids computationally demanding in extended systems with small bandgaps, while in finite systems the rapid decay of semilocal exchange causes errors in quantities sensitive to the long-range potential. Both problems can be addressed by range-separated hybrids which include nonlocal exchange only for some values of the interelectronic separation. Excluding long-range nonlocal exchange in extended systems improves computational efficiency without loss of accuracy, while including full long-range nonlocal exchange in finite systems improves accuracy without loss of efficiency. Both approaches use a significant fraction of nonlocal exchange for intermediate electronic separations. We show that a hybrid functional that uses nonlocal exchange only for this middle range has many advantages, properly describing thermochemistry, reaction barriers, and bandgaps in the same framework.

12:03PM Q13.00005 Molecular Crystals, a test system for weak bonding,\textsuperscript{1}, BERNARD DELLEY, Paul Scherrer Institut Switzerland, TEODORA TODOROVA, Paul Scherrer Institut Switzerland — Intermolecular binding in molecular crystals are due to electrostatic and Van-der-Waals interactions. Crystal parameters are crucially dependent on the accuracy of the electronic model. We investigate sets of molecular crystals, classified by the lowest non-vanishing molecular multipole moment, with density functional theory. We find that certain density functional approximations give an almost surprisingly good description of such lattices, deteriorating only moderately going from molecules with dipole moment, to ones with quadrupole and to even higher symmetry molecules, where finally Van-der-Waals interactions dominate at large distance. For the best performing density functional approximations, even the VdW subset has an error range of calculated lattice parameters comparable to crystals with covalent, ionic or metallic bonds.

\textsuperscript{1}supported under swiss NF grant 200021-109358.
Supported by NSF DMR-0505270 and by the IRG program of New Mexico State University.


12:39PM Q13.0008 Generalized LDA+U+V functional in DFT calculations for covalent systems
VIVALDO CAMPO, MATTEO COCCIONI, Computing and Materials Science Department, University of Minnesota, Minneapolis, MN 55455, USA — In this work, we introduce a generalized LDA+U+V functional that consists in both on-site (U) and inter-site (V) interactions. While V can be straightforwardly obtained from the same linear-response approach used to calculate U [1], its inclusion in the “+U” functional can improve the treatment of systems where electrons tend to localize on molecular states (bonds) rather than on atomic orbitals, and will extend the applicability of this approach to an even broader class of systems. Because of a better treatment of hybridization, this extension also helps avoiding well-known drawbacks of “standard” (atomic) LDA+U such as the exaggerated down-shift of the energy of localized filled orbitals. It thus results in an improved energetic description, which is crucial for studying structural relaxations, chemical reactions and phase transitions. Paradigmatic examples of application of this generalized approach will include diatomic molecules, TM oxides and group-IV solids. ¹ M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005).

12:51PM Q13.0009 Comparative Study of the Performance of DFT B3PW91 for the Prediction of Electronic Properties of Molecules
JASMA BATHAM, PEDRO DEROSA, Louisiana Tech University — Density Functional Theory is a widely used and accepted tool for the prediction of ground state molecular properties. However and despite the fact that the hybrid GGA functional B3PW91 has proven to be successful for many application, its use seems not to be as widespread. In a paper by Zhang and Musgrave the HOMO, the LUMO and the energy difference between the two (HLG), is compared for a set of 27 molecules to the experimental ionization potential (IA), electron affinity (EA), and the lowest excitation energy respectively. The first two are inspired by the Koopman’s theorem that suggests that the HOMO is a good approximation of IP while the negative of the LUMO is an approximation of the -EA. Notably, in the mentioned paper, results for 11 different DFT functional are compared but B3PW91 is not one of them. In this work we compare the performance of B3PW91, to that of B3LYP, also a hybrid functional, and the corresponding non-hybrid GGAs BLYP and BPW91 for the same 27 molecules. For all the cases the 6-311+G** basis set is used. We compare HOMO, LUMO and HLG to the experimental IP, EA, and first excitation energy among the four methods. In addition we formally calculated the IP and EA as the difference in energy between the corresponding ion and the neutral. B3PW91 show at least comparable results to other methods more commonly used.

1:03PM Q13.0010 Relativistic Density Functional Theory Calculations of the Electron Paramagnetic Resonance Parameters for Vanadyl Acetyl Acetonate and Copper Acetyl Acetonate
LAXMAN MAINALI, INDIRA SAHU, KEITH EARLE, Department of Physics, SUNY at Albany — Relativistic density functional theory calculations of electron paramagnetic resonance (EPR) parameters using a variety of basis sets have been computed for the molecular systems Vanadyl acetyl acetone and Copper acetyl acetone using the ORCA program. The basis set dependence of g and A tensor calculations for Vanadyl acetyl acetonate and Copper acetyl acetone were studied using Pople Style and Ahirachs basis sets in Local and gradient corrected functionals (BP86 and PW91) and Hybrid functionals (B3LYP and PW1PW). The PW1PW hybrid functional gives the best values for VO(acac)2 using the TZV basis set and for Cu(acac)2 using the 6-311G(d) basis set. The calculated A values with PW1PW hybrid functional for VO(acac)2 and Local and gradient corrected functional (BP86) for Cu(acac)2, with same basis set (DZ) give better results than previously reported values using the Amsterdam Density Functional Theory (ADF) Software. Our calculated g and A tensor values are in good agreement with the values determined from experiment.

1:15PM Q13.00011 ABSTRACT WITHDRAWN —

1:27PM Q13.00012 Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets
WILLIAM GARBER, DMITRI VOLJA, WEI KU, Brookhaven National Laboratory — A new development of first-principles electronic method will be presented based on direct energy functional minimization and bi-orthogonal wavelet basis set. The employment of bi-orthogonal basis allows systematically controlled accuracy while benefiting from the compact support that allows O(N) algorithms. Furthermore, utilization of the interpolating nature of the wavelet, together with the effectiveness of multi-resolution of wavelet, enables very efficient calculation without compromising accuracy. By avoiding solving eigenvalue equation as in standard Kohn-Sham framework, the method is easily extended to parallel algorithms, and allows simple implementation of various non-local functionals. In case of crystals, our method goes directly as solution of Wannier functions, further utilizing their sparseness. This new development is ideal for easy implementation and accurate systematic benchmarking of various modern functionals, and holds the potential to attack very large systems such as nano-materials.

1:39PM Q13.00013 An implementation of LDA+DMFT within the PAW framework: Application to SrVO3.
BERNARD AMADON, CEA Bruyeres le Chatel, DPTA, France, FRANK LECHERMANN, University of Hamburg, Germany, ANTOINE GEORGES, Ecole Polytechnique, CNRS, France — The combination of LDA and DMFT has been used in the past ten years to understand properties of strongly correlated systems. Different interfaces have been used such as Linear Muffin Tin Orbitals and Maximally Localized Wannier Functions. Such schemes are however restricted to simple systems because the construction of wannier functions is demanding or because another simplification is used (such as the atomic sphere approximation). We present a new implementation of LDA+DMFT, which keeps the precision of the Wannier implementation, but which is lighter. It relies on the projection of Kohn-Sham states over localized orbitals to define the correlated subsystem. We have implemented this method within the Projector Augmented Wave Framework. This thus opens the way to electronic structure calculations within LDA+DMFT for more complex structures. We present an application to SrVO3. The results are compared to calculations done on the Wannier basis and we discuss the features of the total spectral function.
11:15AM Q14.00001 Control of Decoherence of Many-Body Excitations in a Bose-Einstein Condensate. NIR BAR-GILL, EITAN ROWEN, NIR DAVIDSON, Weizmann Institute of Science — In this work we discuss collective, many-body excitations of a BEC, and their decay into the condensate continuum. We measure the excitation spectrum of a BEC loaded into a 1D optical lattice, and the decoherence of these excitations due to Beliaev damping, as a function of the lattice depth. The cause for decoherence is the Beliaev decay of Bogoliubov quasi-particles, both of which (the excitation and decay products) are observable experimentally. The unique structure of the BEC reservoir, which is composed of a continuum of initially unoccupied quasi-particle modes, results from the quantum interference between the hole and particle amplitudes of these modes. This structure can be modified in a well-controlled manner by adiabatically loading the BEC into and optical lattice. Therefore, by changing the depth of the lattice, we can control the decoherence rate of the excitations. Our experimental results are compared to 1D calculations of the Bloch-Bogoliubov theory. We find that the rate of decay is either enhanced or suppressed as a function of lattice depth. These results can be explained in the framework of the general formula for decay, which also accounts for both the quantum zeno and anti-zeno effects. Such control of the coherence time could allow further studies of dynamics and phase fluctuations of this many-body system.

11:27AM Q14.00002 Investigating Universal Few-body Physics based on Bose-Einstein Condensates of Cesium Atoms in Optical Lattices. NATHAN GEMELKE, CHEN-LUNG HUNG, XIBO ZHANG, CHENG CHIN, University of Chicago — We present progress on an experiment designed to investigate universality in few-body systems based on Bose-condensed atoms in optical lattices. In particular, we describe how collapse and revival of matter wave coherence may be used as a sensitive probe for non-binary collisions and correlations. We discuss limitations on the technique due to lattice inhomogeneity and hydrodynamic time-of-flight, and suggest remedies based on Feshbach-mediated control of interactions, and application of spin-echo techniques to matter-wave revival. To reach this goal, we have recently demonstrated Bose-Einstein condensation of $3 \times 10^5$ cesium atoms in a crossed-beam dipole trap. A novel trapping geometry is adopted which allows us to smoothly convert the crossed-beam trap to a single layer of two-dimensional (2D) lattices. The single-layer 2D lattice will allow us to directly monitor the density distribution of atoms and identify domains with different atomic populations.

11:39AM Q14.00003 Temperature effects when adiabatically ramping up the optical lattice. LORE POLLET, ETH Zurich, CORINNA KOLLATH, Universite de Geneve, KRIS VAN HOUCKE, University of Massachusetts - Amherst, MATTHIAS TROYER, ETH Zurich — When atoms are loaded into an optical lattice, the process of gradually turning on the lattice is almost adiabatic. We calculate the entropy in the single band Bose-Hubbard model for various densities, interaction strengths and temperatures using Quantum Monte Carlo. This allows us to draw equi-entropy lines in order to study the adiabatic heating when going from the gapless superfluid phase to the gapped Mott phase. We present results in one and two dimensions for homogeneous and trapped systems. We find that current experiments remain in the quantum degenerate regime, and our theory can reproduce experimental time-of-flight images.

11:51AM Q14.00004 Bose-Einstein condensation and superfluidity in optical lattices and periodic porous media; a path integral Monte Carlo study. ALI SHAMS, HENRY GLYDE, University of Delaware — We evaluate the Bose-Einstein condensate density and the superfluid fraction of bosons in a periodic external potential using Path-Integral Monte Carlo (PIMC) methods. A unit cell containing a potential well is replicated into a lattice along 1D using periodic boundary conditions. The aim is to describe bosons in 1D optical lattice or helium confined in a periodic porous medium. The One-Body Density Matrix (OBDM) is evaluated and diagonalized to obtain the single boson natural orbitals (e.g. the condensate orbital) and the occupation of these orbitals (e.g. the condensate fraction). The superfluid density is obtained from the winding number. We investigate (1) the impact of the periodic external potential on the spatial distribution of the condensate, and (2) the correlation between localizing the condensate into separated parts and the loss of superflow along the lattice. For strongly interaction Bosons, as the well depth increases, the condensate becomes depleted in the wells (depletion by interaction). For weakly interacting bosons, as the well depth increases, the BEC is localized at the center of the wells (tightly binding). In both cases, the localization of the condensate suppresses superflow leading to a superfluid-insulator cross-over. The temperature dependence is investigated and comparison with Hubbard models and experiment is made.

12:03PM Q14.00005 Superfluid-Insulator and Roughening Transitions in Domain Walls. SEBNEM GUNES SOYLER, BARBARA CAPOGROSSO-SANSONE, NIKOLAY PROKOFOV, BORIS SVISTUNOV, University of Massachusetts at Amherst. We have investigated superfluid behavior of one and two dimensional interfaces separating solid domains. The system is described by the hard-core Bose-Hubbard Hamiltonian with nearest-neighbor interaction. We present the analysis of superfluid-insulator transition of the interface based on our quntantum Monte Carlo simulations. We also show that, in one dimension the transition is accompanied by the roughening transition, driven by proliferation of charge-1/2 quasiparticles. The temperature dependence is investigated and comparison with Hubbard models and experiment is made.

12:15PM Q14.00006 Ground state properties of one- and two-component Bose-Hubbard model. SEBNEM GUNES SOYLER, BARBARA CAPOGROSSO-SANSONE, NIKOLAY PROKOFOV, BORIS SVISTUNOV, Physics Department, University of Massachusetts, Amherst. We report results for the ground state properties of the single component Bose-Hubbard model and preliminary results for the two-component system at total unity filling factor. Our study is based on exact quantum Monte Carlo simulations by worm algorithm. We compare our answers with those of existing analytic calculations based on strong coupling expansion and mean field theory. This work was supported by the DARPA OLE program.

12:27PM Q14.00007 Mott-insulator mediated Josephson physics. COURTNEY LANNERT, Wellesley College, SMITHA VISHVESHWARA, University of Illinois, Urbana-Champaign — We investigate the phenomenon of Josephson tunneling between superfluid regions separated by Mott insulating regions in the context of the Bose-Hubbard model. Such systems can be realized when bosons on a lattice close to a commensurate filling are subject to a random potential or when bosons of sufficiently small hopping strength are trapped in an applied confining potential (i.e. in cold-atomic systems). Using a pseudospin approach valid at small t/U (large interaction strength or small hopping), we derive the equations of motion of the system and show that they lead to Josephson coupling between disjoint superfluid regions. We find expressions for the bulk energy and the Josephson tunneling energy and evaluate them numerically for realistic experimental parameters in a radially-symmetric parabolically-confined cold atom system. Partially supported by NSF grant DMR-0605871.
KUEI SUN, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign, COURTNEY LANNERT, Wellesley College — We study the inhomogeneous system of interacting bosons in an optical lattice trap. We focus on the weak tunneling region wherein a condensate is predicted to exist between two Mott insulating phases and we consider the effect of applying a radio-frequency (RF) magnetic field in this region. We find that the RF spectrum for driving transitions from one hyperfine species of bosons to another is markedly different between the Mott insulating phase and the condensed phase. In particular, the former has one resonant peak, while the latter has two peaks which show shifts of the order of the tunneling strength between lattice sites. Our results and analyses provide a means of verifying the existence of the condensate.

12:51PM Q14.00009 Bosons with three-body interactions on optical lattices, STEFAN WESSEL, Stuttgart University — Motivated by a recent proposal on using polar molecules in optical lattices driven by microwave fields to induce strong three-body interactions (H. P. Büchler et al., Nature Physics 3, 726 (2007)), we study the quantum phase diagram of the boson Hubbard model with nearest neighbor three-body repulsion using quantum Monte Carlo simulations. In particular, we consider the case of a one-dimensional system in the hard-core limit, and assess the nature of the phases that appear in this regime. Our exact numerical results are compared to analytical findings based on a bosonization approach to the same model. Extensions to higher-dimensional systems are mentioned.

1:03PM Q14.00010 Supersolidity from defect-condensation in the extended boson Hubbard model.
YU-CHUN CHEN, National Taiwan University, ROGER G. MELKÒ, University of Waterloo, STEFAN WESSEL, Universität Stuttgart, YING-JER KAO, National Taiwan University — We study the ground state phase diagram of the hard-core extended boson Hubbard model on the square lattice with both nearest- (nn) and next-nearest-neighbor (nnn) hopping and repulsion, using Gutzwiller mean field theory and quantum Monte Carlo simulations. We observe the formation of supersolid states with checkerboard, striped, and quarter-filled crystal structures, when the system is doped away from commensurate fillings. In the striped supersolid phase, a strong anisotropy in the superfluid density is obtained from the simulations; however, the transverse component remains finite, indicating a true two-dimensional superflow. We find that upon doping, the striped supersolid transitions directly into the supersolid with quarter-filled crystal structure, via a first-order stripe melting transition.

1:15PM Q14.00011 Bose Hubbard model in the presence of Ohmic dissipation.
DENIS DALIDOVICH, MALCOLM KENNÉTT, Simon Fraser University — We study the zero temperature mean-field phase diagram of the Bose-Hubbard model in the presence of local interactions between the bosons and an external bath. We consider a coupling that conserves the on-site occupation number, preserving the robustness of the Mott and superfluid phases. We show that this interaction with the bath shrinks the size of the Mott lobes, leading to superfluidity around the points where $\frac{n}{\mu/U}$ is integer, even in the absence of hopping between the sites. It also imposes an upper limit on the possible occupation numbers in the Mott phase, $n_{\text{max}}$ which is relatively small. We discuss the role that such a bath coupling may play in experiments that probe the formation of the insulator-superfluid shell structure in systems of trapped atoms.

1:27PM Q14.00012 Incommensurate superfluidity of bosons in the optical lattice of double-well potentials.
VLADIMIR M. STOJANOVIC, Carnegie Mellon University, CONJUN WU, University of California, San Diego, W. VINCENT LIU, University of Pittsburgh, SANKAR DAS SARMA, University of Maryland, College Park — We study the first excited band of the Bose-Hubbard model in a double-well optical lattice, a setup recently experimentally realized by a group at NIST. A unique feature of this system is the two lowest bands being far separated from the higher bands, which leads to a greatly reduced phase space for the decay of bosons initially occupying the first excited band. By calculating the parameters of the Bose-Hubbard model based on the nonseparable optical lattice potential used in the NIST experiments, we estimate that in the most favorable situations the lifetime of bosons in the first excited band can be several orders of magnitude longer than the characteristic time scales associated with nearest-neighbor tunneling. An additional novel feature of this system is that the band-minima of the excited band occur at an incommensurate finite crystal momentum, suggesting a new superfluid state of circulating currents that spontaneously breaks the time-reversal, rotational, and translational symmetries. We discuss possible physical consequences of this unconventional state.

1:39PM Q14.00013 Superfluid-insulator transition in Fermi-Bose mixtures and the orthogonality catastrophe.
GIL REFAEL, Caltech, EUGENE DEMLER, Harvard University — The superfluid-insulator transition of bosons is strongly modified by the presence of Fermions. Through an imaginary-time path integral approach, we account for the statics as well as the dynamical screening effects of the Fermions on the boson's superfluid transition line. We find that an effect akin to the fermionic orthogonality catastrophe, arising from the fermionic screening fluctuations, suppresses superfluidity. We analyze this effect for various mixture parameters and temperatures, and consider possible signatures of the orthogonality catastrophe effect in other measurements of the mixture.

1:51PM Q14.00014 Novel few- and many-body lattice methods for cold atoms.
DEAN LEE, North Carolina State University — We discuss general methods for measuring scattering phase shifts, spin-orbit coupling, and mixing angles for quantum particles on a lattice. We also present many-body lattice results for ground state properties at unitarity and deviations due to finite S-wave scattering length, S-wave effective range, and P-wave scattering volumes.

2:03PM Q14.00015 Cat state production with ultracold bosons in rotating ring superlattices.
ANDREAS NUNNENKAMP, Clarendon Laboratory, University of Oxford, ANA MARIA REY, ITAMP, Harvard University, USA, KEITH BURNETT, University of Sheffield, UK — Ultracold bosons in rotating ring lattices have previously been shown to form cat-like superpositions of different quasi-momentum states. We demonstrate that cat state production in slightly non-uniform ring lattices has several advantages: the energy gap decreases less severely with the number of particles, the sensitivity to detunings from the critical rotation frequency is reduced, and the scheme is not limited to commensurate fillings. We show that different quasi-momentum states can be distinguished in time-of-flight absorption imaging and propose to probe cat-like correlations via the many-body oscillations induced by a sudden change in the rotation frequency.

We acknowledge support from the Rhodes Trust (A.N.), ITAMP (A.M.R.), the Royal Society and the Wolfson Foundation (K.B.).

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Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q15 DMP: Focus Session: Semiconductor Qubit Approaches I Morial Convention Center 207
11:15AM Q15.00001 Spin Dependent Transport in Si/SiGe Few-Electron Quantum Dots
CHRISTIE SIMMONS, University of Wisconsin - Madison — Si/SiGe quantum dots are of interest for quantum information processing due in large part to the existence of spin zero isotopes of both Si and Ge. We present the results of transport measurements and integrated charge sensing in silicon double and single quantum dots.[1,2] We observe two effects arising from spin dependent transport in a double quantum dot. First, and as expected, for one direction of current flow we observe spin blockade – the canonical example of spin-to-charge conversion in transport. In addition, when current flow is reversed, we observe a second effect: strong tails of current extend from the sharp triangular regions in which current conventionally is observed. The presence of these tails is explained by a combination of long spin relaxation times and preferential loading of an excited spin state. We also present charge-sensing measurements of single and double quantum dots using an integrated quantum point contact. The charge sensor signal from single electron tunneling is well correlated with conventional transport through the system. When the tunnel barrier is large and transport through the dot is not measurable, charge sensing remains a viable means to track charge transitions and is used to confirm individual-electron occupation in a single quantum dot. Work performed in collaboration with Nakul Shaji, Madhu Thalakulam, Levente J. Klein, H. Luo, Hua Qin, R. H. Blick, D. E. Savage, M. G. Lagally, A. J. Rimberg, R. Joynt, M. Frieden, S. N. Coppersmith, M. A. Eriksson. Work supported by ARO, LPS, NSF and DOE. (1) Shaji, N. et al. e-print arXiv:0708.0794 (2) Simmons, C. B. et al. Appl. Phys. Lett. 91, 213103 (2007).

11:51AM Q15.00002 Coulomb Blockade in Double Top Gated Si MOS Nano-Structures, ERIC NORDBERG, University of Wisconsin - Madison and Sandia National Laboratories, MALCOLM CARROLL, MIKE LILLY, KENT CHILDS, LISAY TRACY, KEVIN ENG, ROBERT GRUBBS, JOEL WENDT, JEFF STEVENS, Sandia National Laboratories, MARK ERIKSSON, University of Wisconsin - Madison — Recent demonstrations of Pauli blocked transport in Si-based double quantum dots [1,2] have demonstrated that the basic processes involved in spin-to-charge conversion are observable in quantized quantum dots in Si. In this work, we will present results on the fabrication and electrical transport properties of novel double top gated Si MOS nano-structures. Potential advantages include: variable 2DEG density, CMOS compatible processes, and relatively small vertical length scales. A silicon foundry was used for initial processing steps and produced MOS structures with a peak mobility of 12000 cm2/V·s at electron densities of 1×1012/cm2. Resulting structures, demonstrate Coulomb blockade, and we will discuss the effect of different geometries (vertical top gate spacing, and single and double dot designs) on Coulomb blockade in these Si MOS structures. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. (1) Nakul Shaji et al. arXiv:0708.0794v1 (2) H. W. Liu et al. arXiv:0707.3513v1

12:03PM Q15.00003 Dephasing of exchange coupled spin qubits by electron-phonon coupling in Silicon1, XUEDONG HU, University at Buffalo, The State University of New York — Silicon is regarded as one of the most promising host materials for solid state spin-based quantum information processing because of small spin-orbit interaction and the prospect of removing nuclear spins through isotopic purification. However, in a coupled spin system, charge and orbital fluctuations are as harmful to the spin qubits as in other semiconducting materials. Here we explore pure dephasing between the two-electron singlet and triplet states for two exchange-coupled spin qubits in a double quantum dot, with particular attention paid to the multi-valley nature of the silicon conduction band.

1This work is supported by NSA, LPS, ARO, and NSF.

12:15PM Q15.00004 Decoherence and Relaxation in Two-electron Si Quantum Dots, MARTA PRADA, University of Wisconsin Madison, MARK FRIESEN, ROBERT JOYNT — We study the relaxation process for a doubly-occupied silicon quantum dot from an excited (triplet) state to the ground (singlet) state. The dominant mechanism available in absence of an external magnetic field is the hyperfine coupling with nuclei via a virtual state. Since a direct transition is forbidden by energy conservation, (the energy associated with a nuclear spin is three orders of magnitude smaller than that of the electron spin), the change in energy of the electron spin has to be compensated by a lattice vibration, or emission of a phonon. On the other hand, in absence of time reversal symmetry, spin-orbit (SO) admixtures different spin states through the Rashba SO coupling. This leads to a non-vanishing matrix element for the phonon-assisted transition between a singlet and a triplet state, where the phonon provides only energy conservation, potentially increasing the relaxation rate, 1/ΓST. We find relaxation times TST of a few seconds for a 40×40×15nm3 Si quantum dot in a magnetic field of 1T.

12:27PM Q15.00005 Spin-singlet-triplet relaxation times in Si double quantum dots, ANTON VORONTSOV, MAXIM VAVILOV, University of Wisconsin - Madison — Recent observation of spin-sensitive transport in semiconductor quantum dots presents a new way of spin manipulation in nanoscale devices. Spin-flip processes are essential for understanding the potential of these systems. Following experiments by A. C. Johnson et al. Phys.Rev.B 72, 165308 (2005) and N. Shaji et al. [cond-mat/0708.0794] we calculate the relaxation times of different spin configurations in double quantum dots. For two-electron states, we evaluate the effects of leads on the spin-flip transitions, compare these effects with relevant spin-orbit and nuclear spin relaxation mechanisms, and calculate the electric current profile, including structure of the peaks and temperature dependence of the transport in the suppressed (‘valley’) region.

12:39PM Q15.00006 Spin resonance of 2D electrons in silicon MOS structures1, S. SHANKAR, A.M. TYRYSKIN, S. A. LYON, Princeton University — Metal-oxide-silicon (MOS) heterostructures are a well developed technology, but not much is known about the electron spin properties of this system. However the promise of utilizing electron spins in MOS structures as qubits for quantum information processing calls for detailed study of these properties. We have previously reported an ESR signal at g = 1.9999(1) originating from 2D electrons in a MOSFET. The signal arises from mobile 2D electrons at gate voltages above threshold and weakly confined electrons below threshold. The signal intensity for confined electrons follows the expected Curie-like 1/T temperature dependence characteristic of isolated, independent spins. At high electron densities, where the Fermi energy is large compared to the microwave frequency, one might expect a simple Pauli susceptibility temperature dependence. In particular, electron spin susceptibility is expected to become constant at low temperatures. Perhaps surprisingly, we find that below about 4 K, the spin susceptibility decreases as the temperature is lowered. At electron densities from 3×1011 to 10×1011 cm−2, the signal intensity falls by a factor of 5, as the temperature is reduced from 4 to 2 K. A more sophisticated analysis is required to explain the temperature dependence of the mobile 2D electron ESR signal.

1Supported by LPS/ARO

12:51PM Q15.00007 Valley Splitting in Electrostatically Confined Structures at the Si/SiO2 Interface, L.A. TRACY, Sandia National Laboratories, E.P. NORDBERG, University of Wisconsin, K. ENG, M.P. LILLY, M.S. CARROLL, Sandia National Laboratories — Silicon is a promising material for qubits that use the spin degree of freedom for their encoding because of the anticipated long spin decoherence times. Electrostatic confinement of electrons at a Si(100)/dielectric interface splits the 6 fold conduction band degeneracy. However, 2DEGs are found to have a relatively small valley splitting between the two lowest levels, which is smaller than predicted for ideal interfaces. Small valley splitting is undesirable as it may detrimentally impact the spin decoherence time. Recent theory suggests that interface properties (e.g., miscut and disorder) can significantly change the valley splitting. Large splitting of the valley states has recently been observed in nanostructures formed in Si/SiGe heterostructures for which it is believed the electrons sampled a small number of atomic terraces [1]. In this talk, we will discuss valley splitting at a Si/SiO2 interface in both conventional MOSFETs, MOS- heterostructures and their dependence on effects such as interface roughness, fixed charge, trap density and strain. The valley splitting is characterized via activation energy measurements in the quantum Hall regime. [1] S. Goswami et al., Nature Physics 3, 41 (2007). Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE under contract DE-AC04-94AL85000.
Substrate orientation dependence of valley-splitting in Silicon nanostructures | NEERAV KHARCHE, SEONGMIN KIM, School of Electrical and Computer Engineering, Network for Computational Nanotechnology, Purdue University, TIMOTHY BOYKIN, Department of Electrical and Computer Engineering, University of Alabama in Huntsville, GERHARD KLIMECK, School of Electrical and Computer Engineering, Network for Computational Nanotechnology, Purdue University — Si nanostructures are being actively perceived for Quantum Computing (QC) devices where valley-splitting (VS) is an important device design parameter. Si is desirable for QC due to its long spin decoherence times, scaling potential and integrability within the present microelectronic infrastructure. Six-fold degenerate valleys in Si interact with each other in the presence of confinements provided by physical dimensions of the nanostructures, and applied electric and magnetic fields. These interactions can result in very-different splittings depending on substrate orientations and inherently present disorders in nanostructures. Surface morphology of Si is highly dependent on substrate orientations and so is the VS. Such surface irregularities are automatically included in supercell tight-binding calculations due to atomistic nature of the Hamiltonian. VS calculations in the Si nanostructures grown on (100), (110), (111) and high index vicinal surfaces will be presented.

Why the Long-term Charge Offset Drift in Si SET Transistors is Much Better than Metal-Based Ones: TLF Stability | NEIL ZIMMERMAN, WILLIAM HUBER, STUART MARTIN, BRIAN SIMonds, EMMANOUEL HOURDAKIS, AKIRA FUJlWARA, YUKINORl ONO, YASUO TAKAHASHI, HIROSHI INOKAWA, CHRISTIAN HOF, MIHA FURLAN, MARk KELLER, JOSÉ AUMENTADO — The charge offset drift is a long-standing problem in metal-based single-electron tunneling (SET) devices, manifesting as a time-dependent instability. Through a compendium of drift measurements on SET transistors fabricated in five different laboratories, we can show that the drift is endemic in metal-based devices, but is absent in Si-based devices. Given that it is well-known that two-level fluctuators (TLF's) exist in Si devices the question naturally arises: why is the long-term drift so much better in the Si-based devices? Our answer: the TLF's in Si devices are stable over time, thermal cycling, etc., whereas the TLF's in the metal-based devices are unstable, and exist in interacting glass-like state. Following these observations, we have developed a model based on the theory of heat evolution in glasses that quantitatively agrees with the rate of charge offset drift in metal-based devices. Finally, we suggest some particular directions for future fabrication that may eliminate this problem.

Vertically coupled Al and Si SETs for characterization of MOS structures at low temperature | LUYAN SUN, B.E. KANE, Laboratory for Physical Sciences, University of Maryland — Due to impurities and interface states, a silicon metal-oxide-semiconductor field-effect transistor (MOSFET) channel is usually imperfect. A single electron transistor (SET) close to the channel provides a useful probe of some of these imperfections at low temperatures, the regime where Si devices may be used for quantum information processing. We incorporate an Al-AlO\textsubscript{2}-Al SET at the gate of a narrow MOSFET to induce a self-aligned and vertically coupled Si SET at the Si/SiO\textsubscript{2} interface [1]. We use this SET sandwich architecture to probe and identify sources of defect charge motion in MOS structures via a cross-correlation measurement between the two SETs. In particular, we will present preliminary data from these devices to study a single charge defect at the Si/SiO\textsubscript{2} interface. [1] L. Sun, K. R. Brown, and B. E. Kane, Appl. Phys. Lett. 91, 142117 (2007).

Gate control of single-electron spins: a multi-scale numerical simulation approach | SANJAY PRABHAKAR, JAMES RAYNOLDS, State University of New York University at Albany — Among recent proposals for next-generation, non-charged-based spintronics there is the notion that a single electron can be trapped and its spin manipulated through the application of gate voltages (Rev. Mod. Phys. 79, 1217 (2007)). In this talk we present numerical simulations of such Spin Single Electron Transistors (SSET) in support of experimental work at the University at Albany, State University of New York aimed at the practical development of post-CMOS concepts and devices. We use a multi-scale simulation strategy to self-consistently solve the Schroedinger-Poisson equations (with and without exchange-correlation effects) to obtain realistic confining and gating potentials for realistic device geometries. We discuss scaling of the equations in the various sub domains of a finite-element discretization to span the dimensions from the micron scale of the gate structures down the single-electron level. We will discuss the calculation of the gate-tuned “g-factor” for electrons and holes (Phys. Rev. B 68, 155330 (2003)) in electro-statically- and lithographically-defined quantum dots including the Rashba and Dresselhaus spin-orbit interactions computed numerically from realistic wave functions. This work is supported through funding from the DARPA/NRI INDEX center.

Negative-result evolution from continuous noisy measurement of a double-dot spin qubit | RUSKO RUSKOV, VIATCHELAV V. DOBROVITSKI, BRUCE N. HARMON, Ames Laboratory — We consider evolution of a double quantum dot (DQD) two-electron spin qubit that is continuously measured with a linear charge detector (quantum point contact). We identify the regime where a non-unitary negative-result evolution of the qubit emerges due to the fact that the system remains in the (1,1) charge state (each dot is occupied by one electron). In this case, the \(|T_0(1,1)|\) triplet spin state is spin-blocked, and the transition between \(|S(1,1)|\) and \(|S(0,2)|\) states is suppressed by the continuous measurement, due to the quantum Zeno effect. Moreover, unitary evolution between \(|T_0(1,1)|\) and \(|S(1,1)|\) states is induced by the negative-result measurement due to presence of \(|S(0,2)|\) state. We demonstrate that these effects exist for both strong and weak coupling between the detector and the DQD system. They can be observed with present-day technologies and can be used for coherent qubit manipulations complimentary to existing methods.

Atomistic calculation of electronic and optical properties of a single InAs quantum dots | M. ZIELINSKI, M. KORKUSINSKI, Institute for Microstructural Sciences, NRC, Ottawa, Canada, W. SHENG, Department of Physics, Fudan University, Shanghai, China, P. HAVRYLAK, Institute for Microstructural Sciences, NRC, Ottawa, Canada — We present an atomistic tight-binding (TB) theory of electronic structure and optical properties of a single self-assembled InAs quantum dot (SAD). In previous work an effective-bond-orbital model (EBOM) was used to calculate electron and hole states of the SAD. The strain distribution was calculated using the continuum elasticity theory and EBOM was coupled to the strain via the Bir-Pikus Hamiltonian. However, the properties of these multimillion-atom systems are influenced by the presence of crystal facets and the symmetry of underlying zinc-blende lattice. In current work we present a fully atomistic TB model, accounting for the atomistic symmetry, and extended to include d-orbitals for proper treatment of interband/intervalley couplings. Strain is included in the Hamiltonian via Slater-Koster rules and a generalized Harrison law, with the equilibrium positions of atoms calculated using the valence force field method. Coulomb matrix elements are found using the TB functions, and electronic properties of N confined excitons (N=1-6) are determined in the CI approach. Emission spectra of multieexcitons are also obtained. Comparison with the previous approach and the experimental results is presented.

**Wednesday, March 12, 2008 11:15AM - 2:15PM**

Session Q16 DBP DPOLY DFD: Focus Session: Cytoskeletal Dynamics and Cell Motility II
11:15AM Q16.00001 Cell migration through connective tissue in 3-D. BEN FABRY, Department of Physics, University of Erlangen-Nuremberg, Germany — A prerequisite for metastasis formation is the ability of tumor cells to invade and migrate through connective tissue. Four key components endow tumor cells with this ability: secretion of matrix-degrading enzymes, firm but temporary adhesion onto connective tissue fibers, contractile force generation, and rapid remodeling of cytoskeletal structures. Cell adhesion, contraction, and cytoskeletal remodeling are biomechanical parameter that can be measured on single cells using a panel of biophysical methods. We use 2-D and 3-D traction microscopy to measure contractile forces; magnetic tweezer micro electromechanical systems to estimate adhesion strengths, cytoskeletal stiffness and myosin ATP turnover rates; and nanoscale particle tracking to measure cytoskeletal remodeling. On a wide range of tumor cell lines we could show that cell invasiveness correlates with increased expression of integrin adhesion receptors, increased contractile force generation, and increased speed of cytoskeletal reorganization. Each of those biomechanical parameters, however, varied considerably between cell lines of similar invasivity, suggesting that tumor cells employ multiple invasion strategies that cannot be unambiguously characterized using a single assay.

11:51AM Q16.00002 Dynamics of active cellular response under stress. RUMI DE, Weizmann Institute of Science, Israel, ASSAF ZEMEL, University of California, Davis, SAMUEL SAFRAN, Weizmann Institute of Science, Israel — Forces exerted by and on adherent cells are important for many physiological processes such as wound healing and tissue formation. In addition, recent experiments have shown that stem cell differentiation is controlled, at least in part, by the elasticity of the surrounding matrix. Using a simple theoretical model that includes the forces due to both the mechanosensitive nature of cells and the elastic response of the matrix, we predict the dynamics of orientation of cells. The model predicts many features observed in measurements of cellular forces and orientation including the increase with time of the forces generated by cells in the absence of applied stress and the consequent decrease of the force in the presence of quasi-static stresses. We also explain the puzzling observation of parallel alignment of cells for static and quasi-static stresses and of nearly perpendicular alignment for dynamically varying stresses. In addition, we predict the response of the cellular orientation to a sinusoidally varying applied stress as a function of frequency. The dependence of the cell orientation angle on the Poisson ratio of the surrounding material can be used to distinguish systems in which cell activity is controlled by stress from those where cell activity is controlled by strain. Reference: Nature Physics, vol. 3, pp 655 (2007).

12:03PM Q16.00003 Observation of Non-local Mechanical Responses to Locally Applied Forces in Cells using Magnetic Micropost Arrays. CORINNE LAMB, YAOHUA LIU, DANIEL REICH, Johns Hopkins University, NATHAN SNIADECKI, University of Washington, CHRISTOPHER CHEN, University of Pennsylvania — The process of force transduction by living cells is linked to changes in cell shape and function. To study this process in more detail, we have developed a novel force detection device, which can also be used to apply external forces to a cell. Cells are cultured atop an array of micrometer scale elasticostic posts, which act as independent sensors to cellular traction forces. An external force is applied to the adherent surface of the cell via a magnetic torque on a cobalt nanowire embedded in a single post. Results measuring the spatially resolved forces exerted by the cell over time indicate two responses: a sudden or a gradual global relaxation of the cell in response to a single force actuation. In both cases, the subcellular distribution of loss in traction forces was not concentrated near the point of stimulation but occurred instead at discrete locations around the cell’s periphery. Observation of these adaptive non-local responses is potentially important in understanding how external forces are transduced into biochemical regulators of cell function.

12:15PM Q16.00004 Substrate Stiffness Detection by Cellular Stress and Strain. SHANG-YOU TEE, PAUL JANMEY, University of Pennsylvania — Cells can detect the stiffness of their microenvironment and use this elasticity information to perform cellular functions. We grow cells in hydrogels of different stiffness. We embed particles in the hydrogels and measure the traction forces exerted on the hydrogel by tracking particle motions. We correlate these motions to protein dynamics and deduce the stress-strain relationship that cells use to measure elasticity.

12:27PM Q16.00005 Probing Eukaryotic Chemotaxis with Optically Manipulated Biomimetic Microparticles. HOLGER KRESS, CECILE MEJEAN, JIN GYU PARK, TAREK FAHMY, ERIC DUFRESNE, Yale University — Chemotactic cells are able to sense chemical gradients and to move towards the source of a chemical agent. Eukaryotic chemotaxis is an important part of the mammalian immune system and poses many questions about the cell's physical mechanisms to detect, process and respond to external stimuli. While an understanding of the balance between directional and random motion is necessary, few methods for precise, controlled and flexible quantitative cell stimulation are needed to test existing hypotheses. We present such a method which is based on optically manipulated biomimetic microparticles. We are developing colloidal particles that provide controlled release of a chemoattractant. These micro-sources of stimulating agents are positioned with optical tweezers at arbitrary locations close to chemotactic cells in order to apply flexible spatio-temporal stimulation patterns to the cells. We show that chemotactic cell response - directed cell polarization, motility and turning - can be induced by our novel stimulation method. In conjunction with live cell microscopy this method is suitable to study the dynamics of intracellular signaling loops.

12:39PM Q16.00006 Quantifying Dictyostelium discoideum Aggregation. COLIN MCCANN, University of Maryland, PAUL KRIEBEL, CAROLE PARENT, National Institutes of Health, WOLFGANG LOSERT, University of Maryland — Upon nutrient deprivation, the social amoebae Dictyostelium discoideum enter a developmental program causing them to aggregate into multicellular organisms. During this process cells sense and secrete chemical signals, often moving in a head-to-tail fashion called a 'stream' as they assemble into larger entities. We measure Dictyostelium speed, shape, and directionality, both inside and outside of streams, and develop methods to distinguish group dynamics from behavior of individual cells. We observe an overall increase in speed during aggregation and a decrease in speed fluctuations once a cell joins a stream. Initial results indicate that when cells are in close proximity the trailing cells migrate specifically toward the backs of leading cells.

12:51PM Q16.00007 Cell motility as a persistent random walk. SIMON NORTHELYKKE, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany. Department of Molecular Biology, Princeton University, FRANK JULICHER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — We study the stochastic properties of trajectories of individual keratocytes that move on a solid substrate. The distribution of observed velocities exhibits a characteristic maximum at finite speed and a local minimum at zero velocity. This velocity distribution depends on the averaging time during which velocities are measured. To characterize the stochastic properties of the system, we determine the correlations between longitudinal and transverse components of the acceleration with the instantaneous velocity. The experimental data can be captured by a simplified physical description of cell locomotion where random forces act on a system of two elastically coupled elements, one of which is driven forward by an active process, dragging the second behind.

1:03PM Q16.00008 Role of receptor patch geometry for cell adhesion in hydrodynamic flow. CHRISTIAN KORN, ULRICH SCHWARZ, University of Heidelberg — Motivated by the physiological and biotechnological importance of cell adhesion under hydrodynamic flow, we theoretically investigate the efficiency of initial binding between a receptor-coated sphere and a ligand-coated wall in linear shear flow. Using a Langevin equation that accounts for both hydrodynamic interactions and Brownian motion, we numerically calculate the mean first passage time (MFPT) for receptor-ligand encounter. We study how the MFPT is influenced by flow rate, receptor and ligand coverage, and receptor patch geometry. With increasing shear rate, the MFPT decreases monotonically. Above a threshold value of a few hundreds, binding efficiency is enhanced only weakly upon increasing the number of receptor patches. Increasing the height of the receptor patches increases binding efficiency much more strongly than increasing their lateral size. This strong dependence on out-of-plane geometry explains why white blood cells adhere to the vessel walls through receptor patches localized to the tips of microvilli, and why malaria-infected red blood cells form elevated receptor patches (knobs). [1] C. Korn and U. S. Schwarz, Phys. Rev. Lett. 97: 138103, 2006. [2] C. B. Korn and U. S. Schwarz. J. Chem. Phys. 126: 095103, 2007.
1:15PM Q16.00009 Dynamic friction measurements on living HeLa cells, MARC-ANTONI GOULET, MARIE-JOSE`EE COLBERT, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — The interaction of cells with various interfaces, and especially man-made surfaces, is an active field of research. In our experiment we use a micropipette to measure both the friction and normal force as a cell slides across a surface. A thin substrate, coated with Poly-L-Lysine is brought into contact with a HeLa cell. The adjustable substrate motion is used to study the response of the cell at various normal forces and speeds. Analysis of the micropipette provides dynamic measurements of both the friction and normal force. With our novel setup we are able to probe the attachment/detachment process of living cells.

1:27PM Q16.00010 AFM method to study mechanics of biological cells with real brushy surface, IGOR SOKOLOV, SWAMINATHAN IYER, RAVI GAIKWAD, VENKATESH SUBBA-RAO, CRAIG WOODWORTH, Clarkson University — AFM is particularly useful for studying biological systems because it can be used on viable cells directly in biological media. Most of the time, the deformation curves measured with AFM on cells have typical “two layer” behavior. As we see from confocal fluorescent images of cells, the cell surface is not flat and covered by a brush-like structure. Here we describe a simple two-layer model to decouple the force response of these two “layers”, the cell body and brush. In contrast with the existing biological methods, AFM is a highly sensitive technique that can provide precise quantitative data on both lengths and grafting densities of the brush while measured directly on viable cells. Moreover, it allows one to decouple true cell rigidity from the contribution of the brush layer. This novel method can be applied to virtually any kind of cells. Ignoring this layer may result in incorrect values of cell rigidity derived from the AFM measurements. We demonstrate the developed method on the example of cancerous and normal human cervical cells.

1:39PM Q16.00011 Dynamical measurement of the physical properties of single cells, MARIE-JOSE`EE COLBERT, CECILE FRADIN, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — The mechanical response of living cells to external forces has attracted the attention of many researchers. We have developed a new tool that takes advantage of an “L” shaped micropipette to micromanipulate a single cell and put it in contact with an adhesive surface mounted on a translation stage. The spring constant of the micropipette is carefully measured and its deflection is used to apply a calibrated force, and probe the mechanical properties of the cell. As the cell is compressed between the pipette and substrate, dynamical measurements of the elasticity of the cell and the adhesion of the membrane to the substrate are obtained by monitoring the displacement of the micropipette. This technique gives access to real time monitoring of the cell response to a constant applied force, thus exploring the relaxation processes of the cell when subjected to deformation.

1:51PM Q16.00012 Computational modeling of cell-cell adhesion and cell-endothelium peeling, KENG-HWE CHIAM, RAYMOND QUEK, A*STAR Institute of High Performance Computing — We describe the use of computational modeling to study the behavior of cells adhering to one another as well as to the circulatory endothelium. The cells are subjected to shear stress imposed by the circulatory plasma, and may peel from the endothelium as a result. Cells that peel have a higher chance to enter circulation and hence pose a greater threat in cancer metastasis. We use the immersed interface method to model the cells and solve for its biomechanical response. We quantitatively study the peeling dynamics as a function of the cells’ material properties and the surrounding fluid’s dynamics. We show how cell peeling from the endothelium is hampered by its adhesive interaction with surrounding cells. In addition, a larger aggregate of cells, such as a tumor embolus, peels more readily from the endothelium than smaller ones. These results may give us insight into the concept of cancer metastatic efficiency.

2:03PM Q16.00013 Implications of Cytoplasmic Streaming for Intracellular Transport and Micro-scale Mixing, JAN-WILLEM VAN DE MEENT, IDAN TUVAL, DAMTP, University of Cambridge, WIM VAN SAARLOOS, Lorentz Institute, Leiden University, RAY GOLDSTEIN, DAMTP, University of Cambridge — Found in many large eukaryotic cells, particularly in plants, cytoplasmic streaming is the circulation of their contents driven by fluid entrainment from organelles carried by molecular motors at the cell periphery. Streaming has frequently been conjectured to aid in transport and mixing of molecular species in the cytoplasm, and, by implication, in cellular homeostasis, yet no mechanism quantifying this enhancement has been demonstrated. We solve the flow and its associated advection-diffusion equations for the archetypal ‘rotational streaming’ found in Characean algae, where the cytoplasm streams up and down along helical bands on the surface of cylindrical internodal solute, allowing faster uptake and response to changes in external concentration. This effect constitutes a novel example of how high Pecl´ et number flows can facilitate diffusive transport and mixing at the micro-scale.

Wednesday, March 12, 2008 11:15AM - 2:15PM — Session Q17 DBP: Focus Session: Hydrophobic Interactions at Multiple Scales in Biology Morial Convention Center 209

11:15AM Q17.00001 Water, Hydrophobic Interactions, and Polymer Collapse, THOMAS TRUSKETT, The University of Texas at Austin — The collapse of a hydrophobic polymer in water is a basic model for many-body hydrophobic interactions, and it holds promise of providing fundamental insights into biomolecular folding transitions. Here, we discuss simulations that probe the effects of monomer length scale along with the strength of monomer-monomer and monomer-water interactions on the thermodynamics of the hydrophobic polymer collapse transition.

11:51AM Q17.00002 Comparing Nonaqueous against Aqueous Solution on the Basis of Scaled-Particle Theory, HENRY S. ASHBAUGH, Tulane University — Normal hexane is adopted as a typical organic solvent for comparison with liquid water in modern theories of hydrophobic hydration, and detailed results are worked out here for the C-atom density in contact with a hard-sphere solute, rho*G(R), for the full range of solute radii. The intramolecular structure of an n-hexane molecule introduces qualitative changes in G(R) compared to scaled-particle models for liquid water. Also worked out is a revised scaled-particle model implemented with molecular simulation results for liquid n-hexane. The classic scaled-particle model, acknowledging the intramolecular structure of an n-hexane molecule, is in qualitative agreement with the revised scaled-particle model results, and is consistent in sizing the methyl/methylene sites which compose n-hexane in the simulation model. The classic and revised scaled-particle models disagree for length scales greater than the radius of a methyl group, however. The liquid-vapor surface tension of n-hexane predicted by the classic scaled-particle model is too large, though the temperature variation is reasonable; this contrasts with the classic scaled-particle theory for water which predicts a reasonable magnitude of the water liquid-vapor surface tension, but an incorrect sign for the temperature derivative at moderate temperatures. Judging on the basis of the arbitrary condition that drying is indicated when G(R) < 1, hard spheres dry at smaller sizes in n-hexane than in liquid water.
and mixed aqueous solutions provide insights relevant to biological assembly. Chemistries (from hydrophobic to hydrophilic) and lengthscales. These simulations combined with those of folding-unfolding of hydrophobic polymers in water roles in biological and colloidal self assembly processes. More recently, lengthscale dependences and manybody effects in these interactions have received renewed attention. We will present results from theory and molecular dynamics simulations on hydration of and interactions between solutes and interfaces of varying chemistry (from hydrophobic to hydrophilic) and lengthscales. These simulations combined with those of folding-unfolding of hydrophobic polymers in water and mixed aqueous solutions provide insights relevant to biological assembly.

1:39PM Q17.00005 Depletion when Water meets a Hydrophobic Surface, ADELE POYNOR, Allegheny College, STEVE GRANICK, University of Illinois Urbana Champaign, PAUL FENTER, Argonne National Laboratory, IAN ROBINSON, University College London — What happens when water is forced into contact with a hydrophobic surface? Our previous synchrotron X-ray reflectivity experiments (Phys. Rev. Lett., 2006) reported strong evidence for the existence of an angstrom-thick region of low-density at this interface. Here we report fresh experiments in which ethanol, a wetting fluid, is studied at these same surfaces to quantify the contribution from terminal methyl groups on the hydrophobic surface that are invisible to X-rays. The existence of a depletion layer when water meets a suitably hydrophobic surface is confirmed. Better quantification of its thickness emerges.

1:51PM Q17.00006 Profile of the Interface between a Hydrophilic Surface and Water, URSULA PEREZ-SALAS, Argonne National Laboratory, JOHAN STALGREN, Stanford Linear Accelerator Center, CHARLES MAJKRZAK, FRANK HEINRICH, NIST Center for Neutron Research, MICHAEL TONEY, Stanford Linear Accelerator Center, DAVID VANDERAH, NIST — Aqueous interfaces are ubiquitous and play a fundamental role in biology, chemistry, and geology. The structure of water near interfaces is of the utmost importance, including chemical reactivity and macromolecular function. Theoretical work by Chandler et al. on polar-apolar interfaces predicts that a water depletion layer exists between a hydrophobic surface and bulk water for hydrophobes larger than \( \sim 20 \text{mm}^2 \) (a \( \sim 4A \) in radius apolar molecule). Until now, what the interface really looks like remains in dispute since recent experiments give conflicting results: from complete wetting (no water depletion layer) to a water depletion layer. Those experiments that have found a water depletion layer report 40-70% water in the depletion zone: 40 -70% and a width of \( \sim 3A \). However, an alternative interpretation to the profiles exists where no depletion layer is required. By studying hydrophobic SAM surfaces against several water mixtures we obtained the hydrophobic/water profile by phase sensitive neutron reflectivity. With this model independent technique we observe a 2 times wider and drier depletion water layer: 6A thick and 0-25% water. Given the level of disagreement, I will review the topic of immiscible interfaces and show how phase sensitive reflectometry is unique in obtaining nm resolution profiles without fitting bias.

2:03PM Q17.00007 Reconstructing the dynamics of water near a model charged surface using inelastic x-ray scattering, NATHAN SCHMIDT, ROBERT CORIDAN, GHEE HWEE LAI, PETER ABBAMONTE, GERARD WONG, University of Illinois at Urbana-Champaign, WONG RESEARCH GROUP TEAM — Understanding the behavior of water near hydrophobic surfaces is fundamental to many aspects in biology and surface. From high resolution inelastic x-ray scattering measurements of the dynamical structure factor at 3rd generation synchrotron sources, we reconstruct the longitudinal (density) response function of water. We use this data set to investigate how water behaves at polar and non-polar surfaces via linear response theory. Preliminary data on this and how water wets hydrophobic surface patches of different sizes will be presented.
11:39 AM Q18.00003 Improving the Dispersion and Interfaces in Polymer-Carbon Nanotube Nanocomposites by Sample Preparation Choice. CHANG-UK LEE, University of Tennessee, Knoxville, MARK DADMUN, University of Tennessee, Oak Ridge National Laboratory — Polymer nanocomposites composed of poly(styrene-vinyl phenol) (PSVP) copolymers and 5 wt % multi-walled carbon nanotubes (MWNTs) were prepared by three different methods, including melt-mixing and solution casting. The MWNTs were either oxidized to incorporate oxygenated defects or utilized as received. The mechanical properties of the nanocomposites were measured by DMA, and the extent of intermolecular hydrogen bonding between MWNTs and PSVP was quantified by IR. Our DMA results suggest that melt-mixing leads to more stable morphologies of the final nanocomposites than solution casting. Additionally, the IR analysis of the nanocomposites indicates melt-mixing can result in the formation of more intermolecular hydrogen bonding between the MWNTs and PSVP than solution casting, and thus suggests that melt-mixing leads to nanocomposites with more reproducible mechanical properties than solution casting. Our results thus provide guidelines to realize improved morphologies and properties of polymer carbon nanotube nanocomposites by optimizing intermolecular interactions between MWNTs and polymers using processing.

11:51 AM Q18.00004 Enhancing Dispersion and Properties of SWNT-polymer Nanocomposites by Controlled Non-covalent Interactions. DIAS LINTON, University of Tennessee — The enhancement of the dispersion and properties of singlewalled carbon nanotubes in a polymer nanocomposite via non-covalent interaction is studied. 1% w/w SWNT are dispersed in random copolymers of methyl methacrylate and 2-(dimethylamino)ethyl methacrylate (DMAEMA), where the composition of the copolymer varies from 0% to 50% DMAEMA. The resulting nanocomposites indicate the existence of interactions between the carbon nanotube and polymer matrix by a shift of the D* peak position (~2600-2700 cm⁻¹) of the polymer nanocomposite. The copolymer with 30% DMAEMA shows the smallest shift, suggesting that the nanotubes are debundled, where it is expected that this non-covalent interaction originate from the tertiary amino group in DMAEMA by formation of an electron-donor interaction with the SWNT.

12:03 PM Q18.00005 Spectroscopic Investigations on Polypropylene – Carbon Nanofibers Composites. MARCEA CHIPARA, The University of Texas at Pan American, JONES BRIAN, University of Nebraska Lincoln, KAREN LOZANO, JOHN R. VILLAREAL, ALIN CRISTIN CHIPARA, ANNA HERNANDEZ, MAGDALENA DORINA CHIPARA, The University of Texas Pan American, DAVID J. SELLMYER, University of Nebraska Lincoln — Nanocomposites were obtained by high-shear mixing of isotactic polypropylene (Marlex HLN-120-01; Philips Sulmika Polypropylene Compound) with various amounts of vapor grown carbon nanofibers (PR-24AG; Pyrograf Products, Inc) by utilizing a HAAKE Rheomix at 65 rpm and 180 °C for 9 min followed by an additional mixing at 90 rpm for 5 min. Composites loaded with various amounts of vapor grown carbon nanofibers have been prepared. Wide angle X-ray scattering investigations focus on the effect of carbon nanofibers on the crystalline phases of polypropylene and on the overall crystallinity degree of the polymeric matrix. Raman spectroscopy analysis concentrates on D and G bands. X-band electron spin resonance investigations aim at a better understanding of the purity of carbon nanofibers and of the ratio between conducting and paramagnetic.

12:15 PM Q18.00006 Simulation of Electrical Conductivity of Composites Containing Uniaxially-Aligned, Finite Rods above the Percolation Threshold. SADIE WHITE, University of Pennsylvania, BRIAN DIDONNA, LAI-CHING CHOU, TOM LUBENSKY, KAREN WINEY, University of Pennsylvania — Simulations probed the percolation behavior of composites containing isotropic and uniaxially aligned, conductive, cylindrical fillers with aspect ratios of 10, 20, and 80. In addition, the random resistor network model was used to calculate the electrical conductivity of these composites at concentrations above the percolation threshold. The observed trends compare favorably with our experimental results in carbon nanotube and carbon nanofiber polymer nanocomposites. For example, the electrical conductivity is highest when the fillers are slightly uniaxially aligned in both simulation and experimental results. In addition, the critical degree of filler orientational order at which the electrical conductivity abruptly decreases was found to depend on rod aspect ratio along the same trends noted for experimental data. This work represents the first simulations of electrical conductivity above the percolation threshold for oriented and isotropic composites containing permeable, conductive, finite-sized rods, and is pertinent to the rapidly expanding field of polymer nanocomposites.

12:27 PM Q18.00007 Polymer Dynamics in Single Wall Carbon Nanotube / Polystyrene Nanocomposites. MINFANG MU, RUSSEL COMPOSTO, Department of Material Science and Engineering, University of Pennsylvania, USA, NIGEL CLARKE, Department of Chemistry, Durham University, UK, KAREN WINEY, Department of Material Science and Engineering, University of Pennsylvania, USA — Polymer nanocomposites provide access to new regimes of polymer dynamics in which the impenetrable filler particles are comparable to and frequently smaller than the end-to-end distances of the polymer. In this study, single wall carbon nanotubes (SWCNTs) / polystyrene (PS) nanocomposites was prepared by a coagulation method. Rheological properties were measured in the linear viscoelastic regime and tracer diffusion coefficients were determined using an elastic recoil detection (ERD) method. The tracer diffusion coefficient first decreases and then increases with increasing SWCNT loading. Across this same range of filler concentration, the plateau modulus and the cross-over frequency are approximately constant. The transition from decreasing to increasing tracer diffusion corresponds approximately with the onset of rheological percolation and appears to increase with decreasing matrix molecular weight. A model is under development to describe the polymer dynamics is polymer nanocomposites.

12:39 PM Q18.00008 Periodic Patterning of Polyethylene Block Copolymers Directed by Carbon Nanotubes. BING LI, Drexel University, LINGYU LI, The Dow Chemical Company, CHRISTOPHER LI, Drexel University — Periodic patterning on one-dimensional carbon nanotubes (CNTs) is of great interest from both scientific and technological points of view. Although both chemical and noncovalent CNT functionalization have attracted extensive attention during the past decades, very few efforts have been dedicated to periodic patterning on individual CNTs. Recently, we demonstrated using a controlled polymer solution crystallization method to achieve periodically decorated CNTs. Polyethylene (PE) and Nylon 6,6 single crystals were controlled to grow on CNTs, forming a unique nanohybrid shish kebab (NHSK) structure. The periodicity was, however, not uniform because the concentration governed growth mechanism. Here we report improving the regularity of the periodic NHSK structures by employing block copolymers (BCPs), polyethylene-b-ethylene oxide (PE-b-PEO), to produce NHSKs on CNTs. By crystalizing BCP on CNTs via thin film crystallization, periodic structures were generated along CNTs. The characteristic microphase separation of BCP was clearly observed, forming the striking alternating stripes perpendicular to the axes of individual CNTs. Furthermore, by functionalizing the BCP blocks with thiol groups, Au nanoparticles were subsequently immobilized on the BCP domains of the hybrid nanomaterial, replicating the periodic patterns.
12:51PM Q18.00009 Clay dispersion and interaction effects in supercritical CO2 processed polystyrene-clay nanocomposites. • R. KANNAN, R. BELLAIR, M. MANITOU, S. HORSCH, Wayne State University, E. GYLAR, Clemson University — The major challenges in producing high performance nanocomposites are in effectively dispersing the clay layers in the matrix and in promoting interactions at the polymer-clay interface. A novel process exploiting the properties of supercritical CO2 (scCO2) has recently been shown to be an effective means to delaminate clay platelets with or without a polymer matrix present. In this study we demonstrate the ability of scCO2 to exfoliate commercial, organically modified clay and to produce nanocomposites with significantly improved properties. Rheology shows solid-like behavior in loadings as low as 2wt%, and elastic modulus improvements as high as 2.5 orders of magnitude in 5wt% nanocomposites. TEM images indicate a rich morphology for scCO2 processed composites, with a large fraction of dispersed platelets. In contrast, solution blended control samples display much larger tactoids and a lack of individual clay sheets. Unexpectedly, XRD shows a dramatic increase in the peak in specific heat during crystallization. Structural analysis shows that the additive particles are well-dispersed in the polymer matrix—-they are surrounded by both crystalline and non-crystalline chain segments, the relative proportions of which depend on x and y and strongly suppress the peak in specific heat during crystallization. The decrease in chain mobility correlates with lower crystallinity and smaller crystallite sizes. Further, the presence of additive particles also dramatically suppresses the peak in specific heat during crystallization. The degree of enhancement in the properties appears to be not only dependant on the degree of dispersion, but also on how polymer-clay interactions are promoted by the supercritical fluid.

1:03PM Q18.00010 Surface characterization of Laponite-Poly(ethylene oxide) nanocomposite films • EDUARD A. STAFANESCU, IOAN I. NEGULESCU, WILLIAM H. DALY, Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803, BOGDAN C. DONOSE, ANH V. NGUYEN, School of Engineering, The University of Newcastle, Callaghan, NSW 2308, Australia — The aim of the present work is to understand how ionic strength of precursor polymer-clay gels influences the final structure of multilayered nanocomposite films fabricated from such gels. We have prepared three aqueous precursor gels containing 3wt% LRD, 2wt% PEO and 95wt% water, in which the salt concentrations were kept at 0X, 1X and 3X with X = 5.57 * 10⁻⁵ g NaCl/mL. The Laponite (LRD) - PEO multilayered films (LRD60%-PEO40%) were fabricated by manually spreading and drying each gel on a glass slide. Prior to the AFM measurements the polymer-clay composite films were freeze-dried by immersion in liquid nitrogen until they were totally degassed. Frozen samples then fractured and left for additional drying for 24 hours in a desiccator. The imaging procedure employed here is tapping mode AFM. Distinct features were identified on the layered transversal surface of the films, and were attributed to the different salt concentrations in the samples. Addition of salt increases the adhesion and compactness properties of the nanoparticles, as a more uniform side surface can be observed after freeze-fracturing the materials.

1:15PM Q18.00011 Viscoelastic Behavior of Polyhedral Oligomeric Silsequioxane (POSS)-Filled Epoxy Matrices • QINGXIU LI, STEPHEN HUTCHESON, GREGORY MCKENNA, Texas Tech University, KADINE MOHOMED, TAM Instruments-Waters LLC, SINDEE SIMON, Texas Tech University — Large residual stress in fiber-filled thermosetting resin composites is a major technological problem encountered during the development and applications of these materials. Strategies to reduce the residual stress of the composites include lowering the thermal stress coefficient by lowering the product of coefficient of thermal expansion and shear modulus (αG) and/or lowering the thermal pressure coefficient by lowering the product of coefficient of thermal expansion and bulk modulus (αK). Nanoparticles are unique fillers for resins used in composites and generally result in improved moduli and increased linear thermal expansion coefficient (CTE); however, the effect on the thermal residual stresses has not been addressed. This paper develops epoxy/polyhedral oligomeric silsequioxane (POSS) nanocomposites with mitigated residual stress. The effect of functionalized POSS loading on the viscoelastic properties, linear coefficient of thermal expansion, and glass transition temperature of epoxy/POSS nanocomposites is investigated. The outcome of the current study provides fundamental knowledge to the design criteria for nanoparticle-filled polymer matrix composites with mitigated residual stress and high shear properties.

1:27PM Q18.00012 Spectacular Improvements in Toughness of Poly(lactide-co-glycolide), PLG, Nanocomposites • HARIS RETSOS, MSEE CORNELL UNIVERSITY, ITHACA, NY TEAM — Poly(lactide-co-glycolide) (PLG), a biocompatible, biodegradable polymer, was toughened by adding small amounts of surface modified clay nanoparticles. The elongation of nanocomposite during tensile tests is highly increased in comparison with that of the pure polymer, while we observed also an increase in modulus. Electron microscopy, X-ray scattering, rheometry and dielectric spectroscopy were used to investigate the toughening mechanism. It is revealed that multiple crazing occurs in the clay nanocomposite right after the yield point. The fibrils in the crazes have the ability to be significantly extended before fracture, which translates into a dramatic increase in elongation before failure. Rheological studies show that the nanoclay particles act as physical crosslinks that increase the fracture strength of the polymer. Small angle x-ray scattering was used to investigate any orientation of nanoparticles during deformation and their mobility provided by the polymer matrix.

1:39PM Q18.00013 ABSTRACT WITHDRAWN —

1:51PM Q18.00014 Rheological Studies on the Quasi-quiescent Crystallization of Polypropylene Nanocomposites1 • XIA DONG, TONGCHEN SUN, FENGHUA CHEN, KE WANG, QIANG FU, CHARLES C. HAN, State Key Laboratory of Polymer Physics and Chemistry, Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China — Isothermal crystallization of isotactic polypropylene/organic modified montmorillonite binary nanocomposite (IPP/OMMT) and IPP/OMMT/PEOc (poly(ethylene-co-octene)) ternary nanocomposites were investigated by polarized optical microscope, rheometer and scanning electron microscope. The modulus change which accompanying the crystallization growth was observed after freeze-fracturing the materials. We show that sticky interactions between polymers and clay nanoparticles suppress crystallization.

The authors thank the fund support from important project 20490220 of NSFC.

2:03PM Q18.00015 Effect of additive particles on the crystallization of homopolymers • ASHOK DASMAHAPATRA, Chemical Engineering, IIT Bombay and Polymer Division, National Chemical Laboratory, Pune, India, GURUSWAMY KUMARASWAMY, Polymer Division, National Chemical Laboratory, Pune, India, HEMANT NANAVATI, Chemical Engineering, IIT Bombay, India — The effect of additive particles on polymer crystallization has been investigated using lattice dynamic Monte Carlo simulation. Additives are compatible with the polymer matrix (viz. there is an attractive “sticky” interaction between additives and monomers) and, additive particles have the same size as a monomer. Polymer crystallization is strongly influenced by both additive fraction, x and the additive-monomer interaction strength, λ. While increase in x or λ the diffusivity of the polymer chain decreases dramatically. The decrease in chain mobility correlates with lower crystallinity and smaller crystallite sizes. Further, the presence of additive particles also dramatically suppresses the peak in specific heat during crystallization. Structural analysis shows that the additive particles are well-dispersed in the polymer matrix—they are surrounded by both crystalline and non-crystalline chain segments, the relative proportions of which depend on x and λ. We show that sticky additive particles suppress crystallization.

Wednesday, March 12, 2008 11:15AM - 2:15PM — Session Q19 FEd: Physics Education: In and Out of the Classroom Morial Convention Center 211
11:15AM Q19.00001 Changes in Student Models of Electric Current and Electric Potential in Activity-Based Physics1. C. TRECIA MARKES, University of Nebraska – Kearney — With a three-year FIPSE grant, it has been possible at the University of Nebraska at Kearney (UNK) to develop and implement activity-based introductory physics at the algebra level. It has generally been recognized that students enter physics classes with misconceptions about current and potential difference in simple series and parallel circuits. Many of these misconceptions persist after instruction. Pretest and posttest responses on the “Electric Circuit Concept Test” (ECC) are analyzed to determine the models that students use. Responses are divided into expert model (correct answer), one or more student models (approximately equally common incorrect answers), and null model (all other answers) categories. Students are categorized as being in an expert state (mostly expert model answers), a mixed state (a combination of expert model answers, student model answers, and null model answers), or a student state (mostly student model answers). The change (if any) of state is identified for each student. The changes are analyzed to determine the effectiveness of activity-based instruction.

This work was supported by the US DOE’s FIPSE Grant No. P116BS1449.

11:27AM Q19.00002 Do physics undergraduate students understand their strengths and weaknesses? R. MICHALAK, University of Wyoming — Physics and non-physics majors self evaluation and confidence responses to exams in undergraduate physics are analyzed with respect to the students’ actual success in the subject. The confidence was sampled in a variety of frequency and sophistication physics classes before and after the exams were taken. Undergraduate populations fall into two subgroups: Students who do have a general awareness whether they have comprehended a topic and students who have not. The divide is all the more surprising as there are students who excel and have no or little confidence that they do excel and as there are students who fail completely and do not see it coming. There is little change in student’s understanding of their comprehension during a given term or between terms.

11:39AM Q19.00003 Experimenting with the virtual environment Moodle in Physics Education. MARIA INES MARTINS, ADRIANA DICKMAN, Pontificia Universidade Catolica de Minas Gerais — The master’s program in Physics Education at the Catholic University in the state of Minas Gerais, Brazil, includes the discipline “Digital technologies in Physics education.” The main goal of this discipline is to discuss the role of Information and Communication Technology (ICT) in the process of learning-teaching science. We introduce our students to several virtual platforms, both free and commercial, discussing their functionality and features. We encourage our students to get in touch with computer tools and resources by planning their own computer based course using the Moodle platform. We discuss different patterns of virtual environment courses, whose proposals are centered mainly in the students, or teacher-centered or even system-centered. The student is free to choose between only one topic and a year course to work with, since their interests vary from learning something more about a specific subject to a complete e-learning course covering the entire school year. (The courses are available online in the address sitesinf01.pucmg.br/moodle. Participation only requires filling out an application form.) After three editions of this discipline, we have several courses available. We realize that students tend to focus on traditional methods, always preserving their role as knowledge-givers. In conclusion, we can say that, in spite of exhaustive discussion about autonomy involved with ICTs abilities, most of the students used the new virtual medium to organize traditional teacher-centered courses.

11:51AM Q19.00004 Writing and representation in liquid crystal physics research. CHAD WICKMAN, CHRISTINA HAAS, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — Public understanding of science is often shaped by semiotic systems—linguistic, mathematical, graphic, pictorial—deployed in the textual presentation of scientific findings. Nowhere is this more apparent, perhaps, than in recent debates over climate change where non-quantitative communication has played an integral role in shaping public discourse. This is one example of many, but it speaks to the need for research that examines how working scientists disseminate knowledge to expert and non-expert alike. Based on the study of text production in liquid crystal physics research, I will discuss the way in which physicists utilize multiple semiotic systems in their research and publications. Findings suggest that shared meanings are often created through a variety of semiotic forms—from linguistic script to equations to graphs to diagrams—and that these forms offer specific meaning potentials for communicating knowledge to different audiences. Ultimately, I argue that an improved understanding of scientific literacy practices is key to the effective communication of science to various constituencies.

12:03PM Q19.00005 Modeling cell membrane action potentials with RC circuits in a general physics teaching laboratory. M.S. RZCHOWSKI, Physics Dept., University of Wisconsin-Madison — Faculty in the physics department at the University of Wisconsin have been working in collaboration with colleagues in biological sciences to modify a large calculus-based general physics service course populated primarily by students pursuing a career in the biological sciences. Part of this effort involves introducing examples and laboratory experiments that students enter physics classes with misconceptions about current and potential difference in simple series and parallel circuits. Many of these misconceptions persist after instruction. Pretest and posttest responses on the “Electric Circuit Concept Test” (ECC) are analyzed to determine the models that students use. Responses are divided into expert model (correct answer), one or more student models (approximately equally common incorrect answers), and null model (all other answers) categories. Students are categorized as being in an expert state (mostly expert model answers), a mixed state (a combination of expert model answers, student model answers, and null model answers), or a student state (mostly student model answers). The change (if any) of state is identified for each student. The changes are analyzed to determine the effectiveness of activity-based instruction.

12:15PM Q19.00006 Two new experiments in physics based on electrospun polymer nanofibers. NICHOLAS PINTO, University of Puerto Rico – Humacao — Nanoscience and nanotechnology have been the focus of much scientific research worldwide and has great potential in enhancing the way we look at all of our present day electronic devices. If only part of this potential can be made into reality, the results will be phenomenal. Given the vast financial and scientific investment in nanotechnology that is tied to our future, it is important to expose undergraduate Physics and Engineering students to this field of study early in their career. Two experiments related to nanoscience that are currently part of our undergraduate Physics program will be presented. A simple to build and to operate electrospinning apparatus produces conducting polymer nanofibers that are then used in device fabrication. The devices include a nanoresistor and a Schottky nanodiode and yield themselves to straightforward data acquisition and analysis. A modification of the sample chamber can convert one of the experiments into a superabsorbent alcohol vapor sensor.

Work supported by NSF.

12:27PM Q19.00007 Animation of Early Cosmological Models. GREGORY TOPASNA, Virginia Military Institute — Early Greek and renaissance models of the solar system are usually presented as diagrams in most astronomy textbooks. While the intent of such diagrams is to illustrate how these models attempted to account for the motion of the planets, the static nature of the diagrams typically leaves students nonplussed and are often only viewed as mere curiosities. However, animating these earlier models vividly demonstrates the early attempts at cosmology and can reflect some of the accuracies our ancestors were able to achieve. While the complexity of some models may at first seem to make animation a difficult task, we show how such models can be written in a basic mathematical form suitable for animation in FlashMX. While these models are not extremely precise they are accurate enough to show the motion of celestial bodies and have an impact that static images alone can not achieve.
12:39PM Q19.00008 Revitalizing the Advanced Lab Course*, DAVID MARX, Illinois State University — As a hard science, physics is based in observation and experiment. Training of physicists at the undergraduate level must include the recognition that students need a solid foundation in experimental techniques used in the various sub-fields of physics, best practices, and a thorough understanding of data analysis and uncertainty. Recently, recognition of this importance has resulted in the creation of an AAPT task force on the advanced laboratory. An examination of advanced laboratory courses from dozens of universities from across the United States has been conducted by the author, the results of which will be presented. In addition, knowledge gained from this examination has recently been used in revitalizing the Experimental Physics course at Illinois State University.

12:51PM Q19.00009 Teaching a laboratory-intensive online introductory electronics course*, MARK MARKES, University of Nebraska-Kearney — Most current online courses provide little or no hands-on laboratory content. This talk will describe the development and initial experiences with presenting an introductory online electronics course with significant hands-on laboratory content. The course is delivered using a Linux-based Apache web server, a Darwin Streaming Server, a SMART Board interactive white board, SMART Notebook software and a video camcorder. The laboratory uses primarily the Global Specialties PB-505 trainer and a Tenma 20MHz Oscilloscope that are provided to the students for the duration of the course and then returned. Testing is performed using Course Blackboard course management software.

1:03PM Q19.00010 Harnessing the Efficiencies of Industry-Standard Tools in the Electronics Laboratory, MATTHEW VONK, University of Wisconsin River Falls — Powerful and flexible computer based tools have generated impressive productivity gains in the industrial sector. These innovations allow users to simulate the functionality of applications before they are built, to create custom integrated circuits on-the-fly, and to automate data acquisition. While these tools promise similar efficiency gains to student learning in educational settings, many physics classes have been slow to exploit them. This talk will illustrate how a number of these advances have been incorporated into an undergraduate electronics laboratory class. Special emphasis will be given to those tools that are low-cost and intuitive.

1:15PM Q19.00011 The Complete Undergraduate Research Experience Inspired by NASA’s Microgravity University, TIMOTHY RITTER, The University of North Carolina at Pembroke — In a typical undergraduate research experience the student is often assigned a small portion of a more comprehensive endeavor. While they may complete their assigned portion of the project, the larger investigation is usually one that was active prior to the student’s arrival in the lab and will continue once the student has left. What we present here are the results, lessons, and experiences from a multidisciplinary, multicampus, undergraduate microgravity research program. This unique experience requires a team of students to go from the idea stage to final report writing in one year. During the entire process the team is also conducting a vigorous outreach program. The research is conducted as part of NASA’s highly competitive Reduced Gravity Student Flight Opportunities Program. Because of its unique features, we believe our program provides the student with a broader, more comprehensive, and more stimulating research experience than a traditional undergraduate research experience.

1:27PM Q19.00012 Imhotep’s Legacy After School School Science Enrichment Program for African Nova Scotian Learners1, KEVIN HEWITT, Dalhousie Univ., Physics and Atmospheric Science, EMMANUEL NFONOYIM, Dalhousie Univ., BARB HAMILTON-HINCH, Dalhousie Univ., Black Students Advising Centre, MARGO HAMPDEN, Nova Scotia Office of African Nova Scotian Affairs, WAYN HAMILTON, Office of African Nova Scotian Affairs — Imhotep’s Legacy After-School Project (ILASP) is a provincial science and engineering after-school enrichment program established in 2003. It aims to redress the under-representation of African Canadians in postsecondary science studies. ILASP offers African Nova Scotian participants in Grade 7, 8 & 9 important academic and social opportunities at no out-of-pocket cost. It is guided by the fact that young learners will be motivated to regularly attend a program that features high-quality, interactive and fun learning activities that are distinct from but connected to their school curricula. The program is structured to sustain contact with the learners over three years (grade 7, 8, 9) during a crucial phase in their academic careers. University science and engineering students, acting as mentors, foster positive social interactions with young learners and deliver science enrichment activities in a participatory and casual atmosphere. Reasons for the high retention rate among participants will be discussed. Visit our website at http://ilasp.dal.ca/.

1The financial support of the Nova Scotia Dept’t of Education - African Canadian Services Division, Office of African Nova Scotian Affairs, Council on African Canadian Education and the Faculty of Science - Dalhousie University is gratefully acknowledged.

1:39PM Q19.00013 Teaching About Variables in Magnetism to Fifth and Sixth Graders, MICHAEL BIRNKRANT, MATTHEW CATHELL, Material Sci & Eng Dept., Drexel University, Philadelphia, PA, PRISCILLA BLOUNT, JEAN ROBINSON, Martha Washington Elementary School, Philadelphia, PA, ADAM FONTECCHIO, ELI FROMM, Electrical & Computer Eng Dept., Philadelphia, PA — Middle school students are very familiar with using computers, but many are unaware of how a computer stores information. We develop a module to explain how computers store and retrieve information from a hard drive. The module is part of the yearlong NSF GK-12 outreach program between Drexel University and local Philadelphia middle schools. The module complements the variables portion of their science and math curriculum. The module introduces magnetism as well as the link between the physical state of a hard drive and the picture on the screen. This module and others have contributed to improvements both in their classes and on their benchmark exams.

1:51PM Q19.00014 Use of media in introductory physics courses and public outreach, KHAZHGERY SHAKOV, Tulane University, ZALIMGERY SHAKOV, Kabardino-Balkar State University — Making the material presented interesting and exciting for the students has always been one of the main challenges in teaching introductory physics to students who have little or no background in physics (e.g. K-12 or undergraduate college). Many of the traditional teaching strategies consider physical systems (real or fictional) where the “level of distraction” is intentionally minimized or eliminated for the sake of better clarity. While it certainly allows a student to focus on important principles, it often leads to an impression that physics (and science in general) mostly operates with “artificial” systems that are not immediately relevant to everyday life. One of the ways to address this problem is to incorporate different forms of media that would “bring physics to life”. We discuss how one can use fragments of popular movies to enhance students’ interest in the subject.

2:03PM Q19.00015 Analytical Animations: New Views of Physics, DOUG SWEETSER, none — Analytical animation, like analytical geometry before it, opens new ways to look at physics. Systems with both spin 1/2 and spin 1 symmetry can be animated. The groups U(1), SU(2), and SU(3) of the standard model are viewed as animations, and together make visual sense. A new perspective on gamma matrices, a tool used in quantum field theory, is easy to understand based on images. All software used is open source.
11:15AM Q20.00001 Impurity Decoration for Crystal Shape Control: C_{60} on Ag(111)^1, T.J. STASEVICH^2, C.G. TAO, W.G. CULLEN, E.D. WILLIAMS, T.L. EINSTEIN, U. of Maryland. — The decoration of hexagonal Ag/Ag(111) monolayer islands by chains of C_{60}, observed via STM at 300K, dramatically changes their shape and fluctuations. We tune coverage so that a single C_{60} chain fully decorates each Ag island boundary. The C_{60} induced rounding appears due to competing energetic and entropic effects. We estimate the Ag - C_{60} attractions as -0.13 eV and -0.04 eV, respectively. The edge fluctuations are remarkable: 1) C_{60} decoration does not impede the step-edge diffusion (SED) and 2) while the bare-island fluctuations are driven by SED, the decorated island has the signature of non-conserved dynamics, even though the C_{60} remains at the island edge. We suggest that rapidly diffusing Ag atoms randomly attracting the nearby C_{60}s. Generalizations of our model show that both spherical and rectangular decorating molecules will similarly lower the energy of highly-kinked boundaries, leading to similar island shape changes.

1. Work supported by UM NSF-MRSEC grant DMR 05-20471.
2. TJS now at LRBGE, NCI, NIH; CGT at U. Cal. Berkeley
5. T.J. Stasevich et al., submitted.

11:27AM Q20.00002 Optical, Structural and Electrochemical Properties of CeO_{2–Al_{2}O_{3–}SiO_{2}} Thin Films, DURSEN SAYGIN HINCZEWSKI, Istanbul Technical University (I.T.U.), MICHAEL HINCZEWSKI, TUBITAK Bosphorus Univ. Feza Gursey Institute, IDRIS SORAR, ESAT PEHLIVAN, PATMA Z. TEPEHAN, I.T.U., GALIP G. TEPEHAN, Kadir Has Univ. — CeO_{2} thin films can be used as counter-electrodes in electrochromic devices, but have the disadvantage of slow reaction kinetics. Thus research has shifted to composite CeO_{2} films for predicting the properties of the surface-adsorbate complex.

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11:39AM Q20.00003 Organic coverage of the silicon (100) surface: first-principles calculations, GIOVANNI CANTELE, CNR-INFM and University of Napoli “Federico II”, IVO BORRIELLO, University of Napoli “Federico II”, DOMENICO NINNO, CNR-INFM and University of Napoli “Federico II” — Interfacing semiconductor surfaces with organic molecule adsorbates is one of the most challenging aspects of the modern surface and interface engineering. Controlled and periodic surface coverage can have important implications in lots of technological applications, such as molecular sensing, molecular electronics, etc. One of the widely investigated surfaces is the silicon <100>. Such a surface shows a periodic arrangement of silicon dimers (induced by reconstruction) whose bonding has been extensively debated. It turns out that its properties are similar to those of a double carbon-carbon bond, and it is therefore suitable for attaching organic molecules, especially those containing a double bond. In this study we theoretically investigate from first principles the adsorption of ethylene, cyclopentene and a class of its chemical derivatives on the Si <100> surface, discussing the implications in tailoring the surface properties, such as the electron affinity and work function. Each molecular adsorbate induces a dipole layer on the surface, whose magnitude depends on the considered molecular species. Our findings demonstrate that, for this class of systems, it is not enough the knowledge of the isolated molecule properties for predicting the properties of the surface-adsorbate complex.

11:51AM Q20.00004 Ab initio calculations of BaTiO_{3}, PbTiO_{3} and SrTiO_{3} (001) and (111) surfaces, ROBERTS EGLITIS, DAVID VANDERBILT, RUTGERS UNIVERSITY TEAM — We present results of calculations of surface relaxations and rumpling of (001) and (111) surfaces of ATiO_{3} perovskites (A=Ba, Pb, Sr) using a hybrid B3PW description of exchange and correlation. On the (001) surfaces, we consider both AO and TiO_{2} terminations. In the former case, the surface AO layer is found to relax inward for all three materials, while outward relaxations of all atoms in the second layer are found for both kinds of (001) terminations. The surface relaxation energies of AO and TiO_{2} terminations are found to be comparable with each other for all three materials. For (111) surfaces, we consider terminations on a TiO layer, an A layer, or an O layer. The surface relaxation energies for BaTiO_{3}, PbTiO_{3} and SrTiO_{3} (011) surfaces for all terminations are considerably larger than for (001) surfaces. Among the (011) surfaces, the relaxation energy is much larger for the TiO-terminated surface than for the Ba- or Pb-terminated surfaces for the BaTiO_{3} and PbTiO_{3} perovskites. We predict a considerable increase in the Ti-O chemical bond covalency near the (111) surfaces as compared to both the bulk and the (001) surfaces.


12:03PM Q20.00005 Structure of the rutile TiO_{2}(011)-(2x1) surface, NAVID KHORSHIDI, ANDREAS STIERLE, VEDRAN VONK, CLAUS ELLINGER, HELMUT DOSCH, Max Planck Institute for Metals Research, Stuttgart, Germany, ULRIKE DIEBOLD, Tulane University, New Orleans, USA, XUEQING GONG, ANNABELLA SELLonI, Princeton University, Princeton, USA — TiO_{2} has various applications in technology and is one of the most investigated metal oxides. It is used in solar cells and its photocatalytic activity makes an understanding of the structure of diverse surface orientations desirable. Although there are many studies on TiO_{2} surfaces, the (011) surface has been rarely investigated. First principal DFT calculations predict the (011)-(1x1) face to have the third lowest energy and in a Wuiff Construction a large part of the surface is (011) oriented. TiO_{2} nanoparticle exhibit preferentially (011) oriented facets. Therefore a structure model of this surface is required to understand the photocatalytic processes on an atomic scale. We have investigated the TiO_{2}(011)-(2x1) surface using Surface X-Ray Diffraction (SXRD), Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). From our data we are able to derive a novel model for the (011) surface in combination with DFT calculations. The new model has a much lower surface energy than the one suggested previously and fits the X-Ray data very well.

12:15PM Q20.00006 Surface Reactivity, and Lead Sorption of Hydrated Alumina and Hematite Surfaces, SARA MASON, ANNE CHAKA, NIST — It is well known that polarity and structure of oxide surfaces have significant impacts on reactivity. Experimental and theoretical studies at solid-aqueous interfaces have revealed that hydrated oxide surface morphology can vary significantly from surfaces under high vacuum conditions. We apply a combination of density functional theory simulations and ab initio thermodynamics to hydrated structures of α-Al_{2}O_{3} and α-Fe_{2}O_{3} surfaces. While geometrically isostructural in the bulk, these two oxides have sharp contrasts in electronic structure and can have thermodynamically stable surface terminations which differ in both the number and type of exposed functional groups. We use the environmentally relevant interaction of Pb(II) with the hydrated surfaces to explore relationships between reactivity and both surface structure and identity.

12:27PM Q20.00007 Development of the EAM Potential for Fe-C Alloy Systems, BOHUMIR JELINEK, JEFF HOUZE, SUNGHO KIM, AMITAVA MOITRA, LAALITHA LIYAGNE, MARK HORSTMUEYER, SEONG-GON KIM, Mississippi State University — The ab-initio calculations based on density functional theory (DFT) are performed for Fe and C in their ground state crystal structures. Heats of formation are then calculated for different Fe–C alloy compounds. The lattice constant (volume), bulk modulus and shear moduli for cementite are determined from the total energy calculations for bcc Fe and fcc C. The results of the new potential are compared with the results of ab-initio calculations.

1. Work supported by UM NSF-MRSEC grant DMR 05-20471.
2. TJS now at LRBGE, NCI, NIH; CGT at U. Cal. Berkeley
5. T.J. Stasevich et al., submitted.

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12:39PM Q20.00008 Embedded Atom Method (EAM) interatomic potential for Zinc (Zn)

AMITAVA MOITRA, SUNGHO KIM, JEFFRY HOUZE, BOHUMIR JELINEK, LAALITHA LIYANAGE, Dept. of Physics and Astronomy, Center for Advanced Vehicular System, Mississippi State University, MARK F. HORSTEMEYER, Dept. of Mechanical Engineering; Center for Advanced Vehicular System, Mississippi State University, SEONG-ONG KIM, Dept. of Physics and Astronomy; Center for Advanced Vehicular System, Mississippi State University — We developed a new spline-based embedded-atom method (EAM) interatomic potential for Zn by matching forces to those of ab-initio calculations. The material parameters such as cohesive energy, equilibrium atomic volume, and bulk modulus were used to optimize the potential. The applicability of the new potential was demonstrated by performing atomistic simulations for different surfaces. The formation energies, and various point defects were also calculated. The applicability of this EAM potential to the stability analysis of small clusters was also tested.

12:51PM Q20.00009 Calculation of Absorption Energies Using EAM Potential for Al-Mg alloy systems

LAALITHA LIYANAGE1, BOHUMIR JELINEK2, SUNGHO KIM, MARK F. HORSTEMEYER3, SEONG GON KIM4, Center for advanced vehicular system — Spline-based embedded-atom method (EAM) interatomic potentials for Al-Mg alloy systems are developed using existing EAM potentials. The lattice constant, bulk modulus and shear modulus for the alloy are determined to demonstrate the validity of the new potential. The absorption energies of Mg atoms on Al surfaces are also calculated and compared with the results of ab-initio calculations.

1:03PM Q20.00010 Ab initio study of the plutonium dioxide surfaces: role of electronic correlations

GERALD JOMARD, FRANCOIS BOTTIN, Commissariat a l’Energie Atomique — This ab initio study is performed in the framework of density functional theory (DFT) using the projected augmented wave method. Introducing the on-site Coulomb repulsion term U in the calculations, we found equilibration properties of both PuO2 and Pu2O3 in good agreement with experiments. At odds with conventional DFT calculations, these two compounds are no more metallic and recover their insulating behavior with an antiferromagnetic order. As concerns the surface properties of the plutonium dioxide PuO2, we perform an extensive study of eleven (1 x 1) (110), (100) and (111) terminations then compare their thermodynamic stability by computing their surface Grand potential. Whereas conventional DFT calculations predict that a few uncompensated polar terminations can be stable, in the stability domain of the PuO2 compound, the inclusion of the electronic correlations modify significantly these conclusions. We discuss this result by connecting the surface electronic structure to the polar or non-polar character of the termination.

1:15PM Q20.00011 Effect of Mg doping on the Structure and Reflectivity of Alumina surfaces

TIMOTHY PENNYCOOK, Vanderbilt University, JUAN C. IDROBO, Vanderbilt University, SOKRATES T. PANTELIODES, Vanderbilt University, and Oak Ridge National Laboratory, KALMAN VARGA, Vanderbilt University, SOKRATES T. PANTELIODES, Vanderbilt University, and Oak Ridge National Laboratory — Mg is used in the fabrication of Al alloys to increase the strength of the material. In typical applications, a layer of alumina is present on the surface. The high diffusivity and chemical reactivity of Mg means that Mg can migrate from the bulk alloy to the alumina film and the surface, where it can affect the structural and optical properties of the material. The doping of Al alloys with Mg is known to cause “darkening” and affect the coloration of the material. We will report results of first principles density functional theory calculations that explore the segregation modes of Mg in the near-surface region of alumina and the corresponding effect on optical properties, i.e., reflectivity. This work is supported in part by NSF grant DMR-0513048 and ALCOA Inc.

1:27PM Q20.00012 Down the primrose path of dalliance: how iterative structural determination routines for thin films may lead to partial or false solutions

NAJ JUSSEINI, CODRIN CIONCA, Department of Physics, University of Michigan, Ann Arbor, 48109, YIZHAK YACOBY, Racah Institute of Physics, Hebrew University, Jerusalem, Israel, 91904, ROY CLARKE, Department of Physics, University of Michigan, Ann Arbor, 48109 — Iterative methods are frequently used to solve thin film structures. Convergence, however, may terminate at partial or even incorrect solutions. Coherent Bragg Rod Analysis (COBRA), a direct phase retrieval method with minimal iterations, has had recent success with buried interfaces in perovskite oxides and semiconductors. Here, we investigate the role of iterations in COBRA by means of simulations on a model lattice-matched system of PbTiO3 on SrTiO3 with realistic stochastic noise. Out-of-plane atomic displacements were added in various monolayers of the PbTiO3 film. With increasing iterations the positions of the heaviest element (Pb) became more accurate at the expense of the lighter elements – particularly the oxygen sublattices. In addition, the error in the central monolayers of the film decreased while the error at both the film-substrate and film-air interface increased. Our results provide new insights on the influence of uncertainties in measuring subtle structural details at interfaces.

1:39PM Q20.00013 Effect of surface nanostructure on temperature programmed reaction spectroscopy

MICHAEL RIEGER, JUTTA ROGAL, KARSTEN REUTER, Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany) — Using the catalytic CO oxidation at RuO2(110) as a showcase, we employ first-principles kinetic Monte Carlo simulations to illustrate the intricate effects on temperature programmed reaction (TPR) spectroscopy data brought about by the mere correlations between the locations of the active sites at a nanostructured surface. Even in the absence of lateral interactions, this nanostructure alone can cause inhomogeneities that cannot be grasped by prevalent mean-field data analysis procedures, which thus lead to wrong conclusions on the reactivity of the different surface species. The RuO2(110) surface studied here exhibits only two prominent active sites, arranged in simple alternating layers. Yet, the mere neglect of this still quite trivial nanostructure leads mean-field TPR data analysis [1] to extract kinetic parameters that are in error by several orders of magnitude and that do not even reflect the relative reactivity of the different surface species correctly [2].

1:51PM Q20.00014 NMR Evidence of Cage-to-Cage Diffusion of H2 in H2-Clathrates

LASITHA SENADEHERA, MARK CONRADI, Washington University — H2 and heavy-ice at P > 1 kbar and T ~ 250 K form H2-D2O clathrate; four and one H2 may occupy each large (L) and small (S) cage, respectively. In H2-THF-H2O clathrate, H2 occupies singly and only S cages. Previous electronic-structure calculations estimate the barriers for H2 passage though hexagonal and pentagonal faces of cages as ~6 and ~25 kcal/mol, respectively. Our H2 NMR linewidth data reflect random crystal fields from frozen cage-wall D2O orientations. We find dramatic reductions in linewidth starting at 120 K (175 K) for H2-D2O (H2–TDF-D2O) indicating time-averaging of the crystal fields. Assuming Arrhenius behavior, our data imply energies for escape from L (S) cages of about ~4 (~6) kcal/mol. For L cages, the agreement with the calculated (cages were treated as rigid) barrier is reasonable. For H2 in S cages, in H2–TDF-D2O, the extreme disagreement with theory points to another mechanism of time-averaging, reorientations of the cage-wall D2O molecules, as suggested by previous work in TDH-H2O clathrate. Our limited NMR spectra at high T ~145 K in H2-D2O show evidence of distinct resonances from diffusionaly mobile and immobile H2 molecules, as expected.

11:15AM Q21.00001 ”Heterogeneous Electrocatalysis”, ANDRZEJ WIECKOWSKI, University of Illinois, Champaigne — No abstract available.

11:51AM Q21.00002 Tailoring Surface Reactivity of Metal Oxides. ULRIKE DIEBOLD, Department of Physics, Tulane University, New Orleans, LA 70118 — Titanium oxide is receiving continued attention because of its importance as catalyst support, as a material to harvest solar energy for chemical transformations, and as a model metal oxide. In this talk, I will focus on the structure and defects (extrinsic and intrinsic) of less-studied TiO2 surfaces; i.e., rutile (011)-2x1 and anatase (101), and their influence on surface reactivity.

12:27PM Q21.00003 ”Understanding Reaction Pathways on Model Catalyst Surfaces”, WILFRED TSYSOE, University Wisconsin Milwaukee — No abstract available.

1:03PM Q21.00004 Modulating the reactivity of Pt-based catalysts for PEMFC: A First Principles Study, HAI-YAN SU, XIN-HE BAO, WEI-XUE LI, Dalian Institute of Chemical Physics, CAS, Dalian, China — Low-temperature Polymer electrolyte membrane fuel cells (PEMFCs) have been regarded as one of the most promising candidates to produce heat and electricity, especially for electric vehicles or residential co-generation systems. However, the CO poison at the anode and the slow kinetics of the ORR at the cathode for Pt based-catalysts limit its widespread application, which motivated extensive research for more effective catalysts with CO tolerant, highly active and lower Pt loading, and/or highly selective for CO PROX. Density functional theory calculations have been used to screen Pt-based catalysts for PEMFC. It is found that the direct contact with Pt catalysts (so-called Pt-skim) is essential. The reactivity of Pt-skim catalysts towards the oxygen reduction reaction (ORR) and the hydrogen evolution reaction (HER) can be modulated by stepwise increase of Ni contents, which are accomplished by the modification of the reactivity through ligand and geometric effects. The overall reactivity is however balanced by effective adsorption and desorption of adsorbates. Our calculations show that among various Pt-Ni with Pt-skim, Pt3Ni1 is the catalyst with the highest overall reactivity. The present work indicates that it may be a good candidate for CO preferential oxidation (PROX) in excess of the hydrogen.

1:15PM Q21.00005 Surface Site Characterization of COads on Platinum1, PATRICK MCGRATH, AURORA MARIE FOJAS, ELTON CAIRNS, JEFFREY REIMER, University of California - Berkeley — Nuclear magnetic resonance (NMR) spectroscopy is used in conjunction with cyclic voltammetry (CV) to explore the surface chemistry of CO on platinum electrocatalysts. Electrochemically prepared CO ads adsorbed on Pt-skin, Pt3, Pt2, and Pt1 planes are investigated using the 13C-NMR of the adsorbed species resulting from electrochemically adsorbing labeled methanol provides direct insight into the surface electronic structure of the catalysts. We observe a shift in the 13C-NMR spectra associated with different surface preparations. These shifts correlate with the corresponding coverage of the adsorbate on different types of platinum sites. NMR is used to probe the dynamics of these species to elucidate the interaction of the adsorbate with the platinum surface.

1:27PM Q21.00006 Does Pauli repulsion induce the dissociation energy barriers? A first principles study. MASATO ITO, SHIGEYUKI TAKAGI, HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University, JAPAN — We elucidate the origin of the formation analyzing the dissociation process of oxygen molecule on bridge-top-bridge site of Pt(111). The charge state is analyzed by the Bader method together with the spin states of the two oxygen atoms. The charge transfers to the dissociated oxygen molecule from the Au surface. The potential energy variation is in agreement with the energy variation of the separated in distance, charged, and spin polarized oxygen molecules that is calculated with the origin of the formation analyzing the dissociation process of oxygen molecule on bridge-top-bridge site of Pt(111). The charge state is analyzed by the Bader

1:39PM Q21.00007 O2 Dissociative Adsorption on Cu2O(100) with O Vacancies1, DUY LE, SERGEY STOLBOV, TALAT RAHMAN, University of Central Florida — Cu2O surfaces and nanoparticles have been shown to have high activity for CO oxidation [1]. As a result of consumption of the surface oxygen during the CO oxidation process on Cu2O(100), the issue of restoration of the surface composition becomes critical. Through first principles electronic structure calculations of the geometry, activation energy barriers, reaction pathways, and the local densities of electronic states for O2 dissociative adsorption on the Cu2O(100) surface with O vacancies, we show that the healing of oxygen vacancies is accompanied by reconstruction of the surface. Our calculations are based on density functional theory in the generalized gradient approximation and usage of ultrasoft pseudopotential method in the plane wave representation. [1] B. White, M. Yin, A. Hall, D. Le, S. Stolbov, T. S. Rahman, N. Turro, and S. O’Brien, Nano Lett., 6, 2095 (2006).

2:17PM Q21.00008 Modeling the effects of the oxide substrate on O2 dissociative adsorption on Au nanostructures, SERGEY STOLBOV, TALAT S. RAHMAN, University of Central Florida — In this work we apply the density functional theory calculations to explore the mechanism of high reactivity of Au nanoparticles on oxide substrates. We test the idea that the substrate – nanoparticle interaction makes the O2 dissociative adsorption favorable on this system, in contrast to bulk Au, and then the O atoms, so adsorbed, are consumed by reactants for further oxidation. We exploit the observation that the 2-layer Au film on TiO2 displays an exceptionally high reactivity as compared to a monolayer Au film, as well as those with 3 or more layers [1]. We calculate the energy Eads of dissociative adsorption of O2 on the surfaces 1, 2, 3, and 5 Au(111) layer structures in two environments: 1) free standing layers, 2) on TiO2 fragments (modeling a substrate). We find Eads to be negative for the 2- and 3-layer Au films on the “substrate” while it is positive for all other systems under consideration. This result along with the experimental finding [1] point to the O2 dissociative adsorption as being the main mechanism for the observed reactivity of Au nanostructures. Calculated local densities of electronic states and local charges in the system will be presented for further insights into the nature of the effect. [1] M. S. Chen, D. W. Goodman, Science 306, 234 (2004).

Work supported in part by DOE under Grant No. DE-FG02-07ER15842. Computational resources: TeraGrid grant No: DMR050030N.

[1] Work supported in part by DOE under Grant No. DE-FG02-07ER15842.

[2] Work supported in part by DOE under Grant No. DE-FG02-03ER15842.
Adaptable polymer particles that can change geometry, flow characteristics, and adsorption properties upon the stimulation of an environmental change, such as temperature, are of great interest in the fields of materials science and engineering. Georgia Institute of Technology, ALFRED J. CROSBY, Polymer Science and Engineering Department, University of Massachusetts, Amherst

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Theoretical and experimental investigations have been carried out to develop adaptable polymer systems that can respond to changes in their environment. These studies have focused on the development of responsive materials that can alter their properties in response to stimuli such as temperature, pH, or light. The goal is to create materials that can be used in various applications, such as drug delivery systems, sensors, and smart materials. The responsive behavior of these materials is often achieved through the incorporation of stimuli-responsive polymers or the use of responsive building blocks that can change their conformation or state in response to the stimuli.

Acknowledgments: Supported by NSF grant CHE-0626111; the ICSD data is a courtesy from NIST.

11:51AM Q22.00002 In-situ Liquid Volume Measurement of Polymer Films Using Surface Plasmon Resonance, YIBING ZHANG, MOHSEN YEGANEH, Corporate Strategic Research, ExxonMobil Research and Engineering Company — Many physical properties of a polymer in contact with liquid can be markedly affected by the amount of the liquid that can penetrate into the polymer matrix. The liquid accessible volume in a polymer matrix is difficult to determine at elevated temperatures and not possible with simple weight gain measurements. A high sensitivity optical Surface Plasmon Resonance (SPR) technique, which has been widely used in chemical and biomedical applications, was developed for determination of liquid accessible volume in a polymer matrix at both room and high temperatures (up to 150 °C). Experimental results and theoretical calculation are in excellent agreement. Hysteresis in liquid accessible volume as a function of organic liquid was observed when temperatures were cycled between room and high temperatures. The newly developed SPR technique for accessible volume determination has a great potential for in-situ characterization of a polymer matrix in contact with liquid.

12:03PM Q22.00003 Interface and dynamic indentation of crosslinked polyester films, SURESH AHUJA, Xerox Corporation — The nanoindentation technique has drawn much interest recently for both its efficiency and versatility in measuring the mechanical properties of small volumes of materials and thin films. Since the unloading curve of polymers depends not only on the holding time but also on the unloading rate, Hysitron Nanoindenter was used in our investigation of contact deformation of surfaces of polyester and polycarbonate supported on an aluminum substrate. Crosslinked polymers with different gel concentration were produced on aluminum surfaces. Inter-phase plays a crucial role in composites. Stiffening and strengthening rely on load transfer across the interface, toughness is influenced by crack deflection/fiber pull-out, and ductility is affected by relaxation of peak stresses near the interface. Instead of strain softening with indentation depth observed in linear polymers, cross-linked polymers showed strain hardening. The extent of diffusion determines the extent of the interfacial region with the conformation loss of large molecules being higher than that of small molecules. Besides, considering the strain hardening, an increasing stress is required to produce further plastic deformation after the material is strained beyond the yielding point, it is possible to separate the plastic deformation and the visco-elastic deformation and study them individually. Steady state deformation is compared with sinusoidal deformation relatable to differences in Tg from confinement effects. In cross-linked polymers, surface deformation is analyzed a three-layer model consisting of free surface layer, intermediate layer, and interface layer. Molecular relaxation dependence on molecular weight and cross-link density is shown.

12:15PM Q22.00004 Prediction of Zeolite Types Based on Structural Data, M. LACH-HAB, D.A. CARR, I. VAISMAN, E. BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA — Application of knowledge discovery methods in the search of information contained in databases is an emerging field in materials science that plays an important role on facilitating data analysis. In this study we propose a model for identification of the zeolite mineral type based on the topological analysis of the underlying crystal structure. High-throughput generation of topological descriptors is derived from the Delaunay tessellation of zeolite supercells. Based on these descriptors, our Zeolite-Structure-Predictor is trained for classifying zeolite crystals into twenty two different types of minerals and is based on a random forest model constructed with attributes that include tetrahedrality index, in-sphere volume, average edge, frequency of occurrence and probability of oxygen rich selected simplices. The underlying crystal structure data used for this study are included in the Inorganic Crystal Structural Database (ICSD).

Acknowledgments: Supported by NSF grant CHE-0626111; the ICSD data is a courtesy from NIST.

12:27PM Q22.00005 Adaptable Polymer Microsrolls, KYRIAKI KALAITZIDOU, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, ALFRED J. CROSBY, Polymer Science and Engineering Department, University of Massachusetts, Amherst — Adaptable polymer particles can change shape, flow characteristics, and adsorption properties upon the stimulation of an environmental change, such as temperature are of great interest in the fields of materials science and engineering. These studies have focused on the development of adaptable polymer systems that can respond to changes in their environment. The goal is to create materials that can be used in various applications, such as drug delivery systems, sensors, and smart materials. The responsive behavior of these materials is often achieved through the incorporation of stimuli-responsive polymers or the use of responsive building blocks that can change their conformation or state in response to the stimuli.

The method is applicable to any material combination that satisfies the design equations. The materials used in this work are gold/titanium (Au/Ti) and polydimethylsiloxane (PDMS). Initial demonstrations of this responsive control and its impact on properties of the adaptable polymer particles are also presented. These structures combined with their demonstrated reversibility have potential as capsules in drug delivery systems and novel conductive composites.
Ordered block copolymer thin films may have important applications in modern device fabrication. Current characterization methods such as conventional GISAXS have fixed electron density contrast that can be overwhelmed by surface scattering. However, soft x-rays have longer wavelength, energy dependent contrast and tunable penetration, making resonant GISAXS a very promising tool for probing nanostructured polymer thin films. Our preliminary investigation was performed using 290 eV resonant GISAXS on block copolymer films on beam-line 5-2 SSRF, and beam-line 6.3.2 at ALS, LBNL. The contrast/sensitivity of the scattering pattern varies significantly with photon energy close to the C K-edge (∼290 eV). Also, higher order peaks are readily observed, indicating hexagonal packing structure in the sample. Comparing to the hard x-ray GISAXS data of the same system, it is clear that resonant GISAXS has richer data and better resolution. Beyond the results on the A-B diblock copolymers, results on ABC block copolymers are especially interesting.

12:15PM Q22.00007 Orientation Distribution for Thin Film Block Copolymers, RONALD JONES, XIAOHUA ZHANG, SANGCHEOL KIM, ALAMGIR KARIM, NIST, ROBERT BRIBER, Univ. of Maryland, HO-CHEOL KIM, IBM Almaden Research Center — The directed self-assembly of nanostructured films with vertically oriented morphologies is a potential solution for manufacture of next generation data storage platforms, microelectronic devices, and nanoporous membranes. In many of these applications, the distribution of orientation must be tightly controlled to enable pattern transfer. This parameter is expected to depend on factors such as the Flory-Huggins chi parameter, but little data has been reported to date. We present results from tomographic small angle scattering on a series of block copolymer films whose assembly has been directed through solvent annealing. Films of poly(styrene-b-ethylene oxide) are cast as a function of annealing time and their orientation distribution reported. The results provide significant insight into the fundamental limits of line edge roughness and defect control possible using this fabrication technique.

1:03PM Q22.00008 Unusual Domain Morphology in PS-b-PFS Block Copolymer Films, SETH DARLING, MURUGANATHAN RAMANATHAN, Argonne National Laboratory, ELIZABETH NETTLETON, University of South Dakota — Gaining control over the structure and order of self-assembled domains is critical to the success of bottom-up fabrication methodologies. We focus on the self-assembly of polystyrene-block-poly(ferrocenylmethylsilane) block copolymers (PS-b-PFS). Thin films microphase separate to form nanoscale PFS cylinders within a PS matrix. Traditionally, order in such films is improved using thermal annealing, which has drawbacks including time requirements and possible thermal degradation. In this work, solvent annealing has been used, sometimes in concert with thermal annealing, to gain control over the microphase domain orientation. In addition to orientational control, novel domain morphologies have been observed. Thermochemical techniques and AFM and TEM imaging have been utilized to characterize these materials. Because of the comparatively high etch resistivity of the PFS block, this block copolymer holds potential in lithographic patterning of nanowires, nanopillar arrays, and nanofluidic channels. Some initial patterning results will also be presented.

1:15PM Q22.00009 Using Functional Small Molecules to Control Self-Assembly and Patterning in Block Copolymer Thin Films, C. GERALDINE BAZUIN, DAVID GASPARD, XIMIN CHEN, DAMIEN MAURAN, ROBERT E. PRUD'HOMME, CHRISTIAN PELLERIN, University of Montreal — Self-assembled thin films of block copolymers constitute an elegant means to obtain nanopatterns and nanotemplates on surfaces. Here, we demonstrate how interacting small molecules can be used to control the morphology of dip-coated block copolymer films. Such films obtained from THF solutions of styrene-4-vinylpyridine block copolymers (PS-b-PVP, ca. 29 wt percent VP) and naphthol (NOH), which hydrogen bonds to PVP, yield nanopatterns of quasi-hexagonally ordered nodules of PVP+NOH in a PS matrix. Washing in methanol removes the small molecules, leaving functional PVP-lined nanopores in the film. These nanopores are receptor sites for molecules with desired properties. In contrast, naphthoic acid (NCOOH), which differs from NOH only by the hydrogen-bonding group, leads to fingerprint morphology under the same initial dip-coating conditions. By changing the conditions, in particular reducing the dip-coating speed sufficiently, the fingerprint morphology can be converted to quasi-hexagonal. Reflection-absorption infrared spectroscopy indicates that the proportion of small molecule incorporated into the dip-coated film is about half that found in solution for both NOH and NCOOH.

1:27PM Q22.00010 Combinatorial Studies of Free Surface Effects on Block Copolymer Thin Films, THOMAS EPPS, JULIE LAWSON, THOMAS SCHERR, University of Delaware, MICHAEL FASOLKA, NIST, Polymers Division — To employ block copolymers for many nanoscale templating applications, it is essential to understand how the interfacial interactions originating from the substrate and free surface in ultrathin (∼nm) films affect block copolymer morphologies. In this work, we manipulated the free surface interactions of poly(styrene-b-isoprene-b-styrene) and poly(styrene-b-ethylene oxide) thin films using solvent vapor gradient libraries. These libraries were created using fluorinated acrylate microfluidic devices consisting of a two-input solvent vapor mixing tree and several discrete solvent vapor flow channels. Areas of the thin films exposed to vapor flowing through the channels were subsequently examined by AFM. Analysis along the discrete vapor gradients showed the expected results for the channels at the extremities (representing the approximately single component vapor streams); however, the channels at intermediate vapor compositions show time-dependent nanostructure behavior that was a function of both vapor composition and distance along the channel.

1:39PM Q22.00011 Self-assembly of Cylindrically Confined Block Copolymers in Core-Shell Electrospun Fibers, MINGLIN MA, GREGORY RUTLEDGE, Chemical Engineering, MIT — We report the development of electrospun fibers with internal nanostructure by two-fluid coaxial electrospinning of block copolymers. Microphase separated morphologies with a long-range order were obtained by electrospinning two-fluid coaxial block copolymers on beam-line 5-2 SSRF, and beam-line 6.3.2 at ALS, LBNL. The contrast/sensitivity of the scattering pattern varies significantly with photon energy close to the C K-edge (∼290 eV). Also, higher order peaks are readily observed, indicating hexagonal packing structure in the sample. Comparing to the hard x-ray GISAXS data of the same system, it is clear that resonant GISAXS has richer data and better resolution. Beyond the results on the A-B diblock copolymers, results on ABC block copolymers are especially interesting.

1P1PM Q22.00012 A Generalized Method for the Preparation of Neutral Brushes from Homopolymer Mixtures, SHENGXUAN JI, GUOLIANG LIU, Department of Chemical & Biological Engineering, University of Wisconsin-Madison, FAN ZHENG, FRANZ HIMPSEL, Department of Physics, University of Wisconsin-Madison, PAUL NEALEY, Department of Chemical & Biological Engineering, University of Wisconsin-Madison — We demonstrate a new, generalized approach for the formation of neutral surfaces that uses a ternary blend of hydroxyl-terminated homopolymers A-OH and B-OH and a low MW A-b-2VP block copolymer. The presence of the block copolymer effectively homogenizes the A/B homopolymer mixture before the homopolymers are grafted onto the substrate, thereby preventing macroscopic phase separation of the homopolymer mixture, and maintaining chemical neutrality over the length scales necessary for the self-assembly of block copolymer microdomains. The grafting ratios of the two homopolymers were varied simply by changing the blend ratios. Neutral compositions for P(S-b-MA) and P(S-b-2VP) were located using this binary homopolymer mixture strategy.
2:03PM Q22.00013 Centrifugal adhesion balance (CAB): A novel surface characterization technique, RAFAEL TAMDOR, LAN DANG, AISHA LEH, PRASHANT BAHAHADUR, KUMUD CHAURASIA — Drop lateral adhesion to a surface and the condition for drop sliding along a surface are key issues in many disciplines including biophysics, environmental science, fluid dynamics and agriculture. Yet, to date, except for the tilt stage method, which is extremely limited in range of forces, there is no systematic experimental instrumentation to measure the forces required for drop sliding. We present a new instrument that uses centrifugal forces to slide any drop along a surface. Beyond extending the range of measurable drop-surface interaction, the instrument enables decoupling of some parameters that are bound to be coupled with the simple tilt stage method. Specifically the tilt stage method has two variables varying at the same time: the lateral and normal forces. This violates a fundamental principle of experimental science which leads to obscured understanding of surface characteristics. The CAB avoids this problem.

Wednesday, March 12, 2008 11:15AM - 1:39PM
Session Q3 DMP GMAG: Focus Session: Bilayer Manganites Morial Convention Center 215

11:15AM Q23.0001 Doping dependence of the bilayered colossal magnetoresistive manganites La(2-x)Sr(1+2x)Mn(2)O(7): Angle Resolved Photoemission studies1, NORMAN MANNELLA, University of Tennessee - Knoxville, KIYOHISA TANAKA, SUNG-KWAN MO, Advanced Light Source - Berkeley, ZHI-XUN SHEN, Stanford University — We have measured the doping dependence of the bilayer colossal magnetoresistive manganites La(2)Sr(1+2)Mn(2)O(7) with Angle Resolve Photoemission (ARPES). Our measurements reveal profound differences in the spectral features depending on the doping levels. Surprisingly, the spectra corresponding to x = 0.4 exhibit more similarities to those corresponding to x = 0.6 than the ones with x = 0.36 and x = 0.38. Further aspects of these data in relation to the physics of layered manganites will be discussed.

1DOE Office of Basic Energy Science, Division of Material Science, under contracts DE-FG03-01ER45929-A001 and DE-AC03-76SF00515

11:27AM Q23.0002 Non-monotonic Fermi surface geometry and its correlation with real-space ordering in the bilayer magnetoresistive oxide La(2−x)Sr(1+2x)Mn(2)O(7), ZHE SUN, J.F. DOUGLAS, Q. WANG, Department of Physics, University of Colorado, Boulder, CO 80309, USA, Y.D. CHUANG, A.V. FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, H. LING, S. SAHRKORPI, B. BARBIELLINI, R.S. MARKIEWICZ, A. BANSIL, Department of Physics, Northeastern University, Boston, MA 02115, USA, H. ZHENG, J.F. MITCHELL, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, D.S. DESSAU, Department of Physics, University of Colorado, Boulder, CO 80309, USA — Angle-resolved photoemission spectroscopy was used to study the Fermi surface and nesting effects for a wide range of doping levels (x) of La(2−x)Sr(1+2x)Mn(2)O(7). While band structure calculations indicate a monotonic trend in the size of each piece of the Fermi surface, our data indicates non-monotonic trends which are consistent with the evolution of the charge modulations, unequivocally confirming the direct connection between the nesting and the charge correlation vectors. This may be classified as a key example of a system with a strongly k-dependent self-energy.

11:39AM Q23.0003 Doping evolution of bilayered colossal magnetoresistive manganites: bilayer splitting and c-axis coupling, CHRIS JOZWIACK, Department of Physics, UC Berkeley, JEFF GRAF, Materials Science Division, LBNL, SHUYUN ZHOU, Department of Physics, UC Berkeley, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, LBNL, HONG ZHENG, Materials Science Division, ANL, JOHN MITCHELL, Materials Sciences Division, ANL, ALESSANDRA LANZARA, Department of Physics, UC Berkeley; MSD LBNL — We present a detailed momentum, doping and temperature dependent study of the electronic properties of bilayer manganites, La(2−x)Sr(1+2x)Mn(2)O(7), by means of angle-resolved photoemission spectroscopy. In particular, we will address both the in-plane bilayer splitting, as well as the out-of-plane band, as a function of doping. We will discuss possible implications for the role of inter-plane coupling in the CMR manganites.

11:51AM Q23.0004 Calculated properties of the La(2−x)Sr(1+2x)Mn(2)O(7) bilayer manganites, 0.30 ≤ x ≤ 0.501, ROLANDO SANIZ, ARTHUR FREEMAN, Northwestern University, MICHAEL NORMAN, Argonne National Laboratory — The low temperature properties of the La(2−x)Sr(1+2x)Mn(2)O(7) 0.30 ≤ x ≤ 0.50 bilayer manganites have been studied in the past using a host of experimental techniques in order to understand the outstanding properties they exhibit. To complement these investigations, we present a systematic study of their calculated ground state properties as a function of doping level, using the highly precise full-potential linearized augmented plane wave (FLAPW) method2 and focusing on magnetic order and optical and transport properties. Our results, which are in very good agreement with experiment in several respects, underline the correlation between the structural and orbital degrees of freedom and also shed light on many of the unexpected behaviors at low temperature in angle-resolved photoemission spectroscopy, optical conductivity, and resistivity measurements.

1Supported by the DOE (DE-FG02-88ER45372 and DE-AC02-06CH11357).

12:03PM Q23.0005 Magnetic State of La(1.36)Sr(1.64)Mn(2)O(7) Probed by Magnetic Force Microscopy1, JUNWEI HUANG, CHANGBAE HYUN, TIEN-MING CHUANG, JEEHOON KIM, ALEX DE LOZANNE, J.B. GOODENOUGH, J.S. ZHOU, U Texas at Austin, JOHN MITCHELL, ANL — We have investigated the evolution of the ferromagnetic (FM) domain structure of a single-crystal La(1.36)Sr(1.64)Mn(2)O(7) with temperature and external magnetic field by using low-temperature magnetic force microscopy. We observed that theFM domains form stable treelike patterns with out-of-plane magnetization below 65 K. As the temperature increases, the FM domains begin to change gradually. Around 88 K, the magnetization changes from the out-of-plane to an in-plane direction. The in-plane FM domains almost completely disappear near the Curie temperature of this sample (Tc ≈ 110 K). Interestingly, the evolution of the FM domain patterns with temperature was seen to coincide with the change in resistivity. We also observed large changes in the magnetic structures upon thermal cycling. We concluded that the formation of FM domains is determined by the competition between the magnetostatic energy and domain-wall energy and is also associated with the 2D character of the system.

1Supported by NSF DMR-0308575 (AdL).
12:15PM Q23.00006 Thermal Expansion, Heat Capacity and Magnetization Measurements of La$_1.25$Sr$_{1.8}$Mn$_2$O$_7$†, RICHARD K. BOLLINGER, J. J. NEUMEIER, Montana State University, H. ZHENG, J. F. MITCHELL, Materials Science Division, Argonne National Laboratory — La$_1.25$Sr$_{1.8}$Mn$_2$O$_7$ is a bi-layered ferromagnet of perovskite structure with two dimensional magnetic and electrical properties. In this presentation, we will show measurements of the specific heat, magnetization, and thermal expansion for single crystalline La$_1.25$Sr$_{1.8}$Mn$_2$O$_7$ in the temperature range 300 K < T < 5 K. The thermal expansion of this tetragonal crystal along the a and c directions will be presented, the anisotropy will be discussed, and the critical behavior near the magnetic transition will be evaluated.

†This material is based upon work supported by the US DOE (DE-FG-06ER46269) and NSF (DMR-0504769).

12:27PM Q23.00007 Thermal conductivity of layered La$_1.2$Sr$_{1.8}$Mn$_2$O$_7$, FILIP RONNING, Los Alamos National Lab, NAMJUNG HUR, NOBUYUKI KURITA, J.D. THOMPSON, ROMAN MOYSHOVICH — La$_1.2$Sr$_{1.8}$Mn$_2$O$_7$ has many similarities to underdoped cuprates: highly anisotropic transport, strong disorder in a charge reservoir layer, and even claims for Fermi arcs. Thus we measured the thermal and charge transport of this system to examine whether the Wiedemann-Franz law is violated in La$_1.2$Sr$_{1.8}$Mn$_2$O$_7$. The work focuses on the elastic properties of Ca$_2$RuO$_4$.

12:39PM Q23.00008 Temperature Dependent Raman Scattering in Layered Manganites, RAJEEV GUPTA, Department of Physics and Materials Science Programme, Indian Institute of Technology, Kanpur 208016, India, D. N. PATEL, S. L. GUPTA, Department of Physics, Indian Institute of Technology, Kanpur 208016, India — La$_2$MnO$_4$ is a perovskite system built up of New York — 99Ru Mössbauer Effect and magnetic measurements have been made on an enriched 99Ru sample of SrRu$_{0.06}$Mn$_{0.94}$O$_2$ which are compared with a series of measurements on compounds SrRu$_2$Mn$_{1-x}$O$_3$ made with natural Ru completed earlier. SrRu$_2$Mn$_{1-x}$O$_3$ is an antiferromagnet for x<0.06 and a ferromagnet for x>0.9. The change from the ferromagnet to the antiferromagnet is accompanied by a change in the hyperfine magnetic field from 420 K with saturation magnetizations depending on the degree of Fe$_{1+}$ lattice parameters are to be quite unusual and reflects the rich phase diagram of these materials. Almost all measured Ca$_2$RuO$_4$ and Re are ordered in a rock-salt type configuration, was prepared at a high pressure (6GPa) and high temperature (1000 C) condition. The crystal structure determined by the synchrotron X-ray powder diffraction was centrosymmetric with a space group I4/m. The critical behavior near the magnetic transition will be evaluated.

12:51PM Q23.00009 Optical Measurements of Transition from Insulator to Metallic Phases in LaxMnO$_3$: Evidence for Mixed Phases Below T_p, MICHAEL DELEON, PENG GAO, TREVOR A. TYSON, Physics Department, New Jersey Institute of Technology, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, CATHERINE DUBOURDIEU, LMGP-Minatc, France — Infrared measurements were conducted over the range 100 to 8000 cm$^{-1}$ on film of LaxMnO$_3$ ($x<0.8$). From these measurements we determined the temperature dependent conductivity, the effective number of carriers and the frequency dependence of specific phonon modes. The Drude model conductivity matches well with the measured DC resistance measurements. The bulk magnetization noset and resistance peak coincide near 25 K lower in temperature and saturates at 200 K. This indicates that a significant volume of the insulating phase exists below Tp.

This research was funded by NSF DMR-0512196, NSF INT-0233316, and CNR/NSF project No.14550.

1:03PM Q23.00010 Experimental Evidence for an Energy Gap in the Magnetic Insulator SrRu$_{0.06}$Mn$_{0.94}$O$_2$, M. DEMARCO, D. COFFEY, Dept. of Physics, Buffalo State College, NY 14222, B. DABROWSKI, S. KOLESNIK, M. MAXWELL, Dept. of Physics, Illinois Institute of Technology, Chicago, IL 60616. — The only copper-free superconductor isostuctural to the cuprates. Among the doped varieties of SrRuO$_3$, the Ca$_2$Sr$_{1.8}$Mn$_2$O$_7$ is an antiferromagnet for x=0.06 and a ferromagnet for x>0.9. The change from the ferromagnet to the antiferromagnet is accompanied by a change in the hyperfine magnetic field from 33T to 50T at 4.2K and also an isomer shift from a +4 to close to a +5 charge state. The measurements of the hyperfine field as a function of temperature show a change from 50T at 4.2K to 40T at 300K. Since the Néel temperature is about 160K for this compound, these small changes indicate that the thermal excitation of spin waves, which lead to the decrease of the hyperfine field with temperature, are strongly suppressed by a gap of order 100K in the spin wave spectrum. This indicates the presence of strong magnetic anisotropy in the material.

This work was supported by the USDOE(DE-FG02-03ER46064) at BSC and by the NSF(DMR-0302617) at NIU.

1:15PM Q23.00011 Elastic properties of the transition metal oxides Ca$_2$-$_x$Sr$_x$RuO$_4$, YANBING LUAN, VEERLE KEPPENS, The University of Tennessee, RONGYING JIN, DAVID MANDRUS, Oak Ridge National Laboratory, THE UNIVERSITY OF TENNESSEE TEAM, OAK RIDGE NATIONAL LABORATORY COLLABORATION — Layered perovskite ruthenates have attracted considerable interest since the discovery of superconductivity in Sr$_2$RuO$_4$. Among the doped varieties of SrRuO$_3$, the Ca$_2$Sr$_{1.8}$Mn$_2$O$_7$ series is heavily studied, as it connects the Mott insulator Ca$_2$RuO$_4$ with the superconductor Sr$_2$RuO$_4$ and exhibits a variety of physical properties. The current work focuses on the elastic properties of Ca$_2$-$_x$Sr$_x$RuO$_4$ Resonant Ultrasonic Spectroscopy (RUS) has been used to study the elastic response of the samples, and results are presented for single crystals with x = 0.2, 0.3, 0.4, 0.5, 1, 1.5, 1.9 and 2.0. The temperature-dependence of the elastic behavior is found to be quite unusual and reflects the rich phase diagram of these materials. Almost all measured Ca$_2$Sr$_{1.8}$RuO$_4$ samples show a soft phonon mode at low temperatures, which is believed to be associated with the dynamics of the RuO$_6$ octahedra.

1:27PM Q23.00012 Synthesis and Physical Properties of Double Perovskite Pb$_2$FeReO$_6$, KOUSUKE NISHIMURA, MASAKI AZUMA, MIKIO TAKANO, YUICHI SHIMAKAWA, Inst. Chem. Res., Kyoto Univ. — A double perovskite Pb$_2$FeReO$_6$, in which Fe and Re are ordered in a rock-salt type configuration, was prepared at a high pressure (6GPa) and high temperature (1000°C) condition. The crystal structure determined by the synchrotron X-ray powder diffraction was centrosymmetric with a space group I4/m with the Pb$^{2+}$ ion on the A-site. The lattice parameters are a = 5.6159(1) Å and c = 7.9455(3) Å. No structural transition to a lower symmetry was observed down to 23 K. The resistivity showed semiconducting behavior. This compound exhibited a ferrimagnetic transition at 420 K with saturation magnetizations depending on the degree of Fe$^{3+}$/Re$^{5+}$ ordering controlled by the cooling rate after the heat treatment.

Wednesday, December 12, 2008 11:15AM - 2:15PM – Session Q24 DMP: Focus Session: Transport in Nanostructures V: Optics, Mechanics, and Networks Morial Convention Center 216
11:15AM Q24.00001 Simultaneous measurements of single-molecule electrical conduction and Raman response, DANIEL WARD, NAOMI HALAS, DOUGLAS NATELSON, Rice University — Electronic conduction through single molecules is affected by the molecular electronic structure as well as by other information that is extremely difficult to assess, such as bonding geometry and chemical environment. The lack of an independent diagnostic technique has long hampered single-molecule conductance studies. We report on simultaneous measurements of single molecule electronic conduction and Raman response in a nanogap geometry using paramercaptoaniline. The measurements show strong correlations in the time variation of the conductance and the Raman spectrum. The Raman changes include "blinking", spectral diffusion, and changes in Raman mode structure. Conduction in nanogaps is known to be dominated by a single or at most a few molecules, demonstrating the correlated Raman response is also single molecule in nature. These observations establish that multimodal sensing of individual molecules is possible in dense mass-producible nanostructures.

11:27AM Q24.00002 Local luminescence characterizations of ZnO nanostructures and their electrical transport characteristics, JI-YONG PARK, YOUNG MU OH, KYUNG MOON LEE, Ajou University, KYUNG HO PARK, Korean Advanced Nanofab Center, YOUNG CHUL KIM, Y.H. AHN, SOONIL LEE, Ajou University — Local luminescence characterizations using cathodoluminescence (CL) emissions from individual ZnO nanostructures with diameters of 30-100 nm are investigated to correlate their optical and electrical properties. Two types of ZnO nanostructures with high and low light carrier densities are identified from electronic transport measurements and concomitant CL characterizations. The results demonstrate that local luminescence characterizations can provide information about inhomogeneities in electrical and optical properties among ZnO nanostructures.

11:39AM Q24.00003 Transport properties of a novel molecular rotor, MEI XUE, K.L. WANG, SANAZ KABEHEI, JEFFREY I. ZINK, UCLA — Rotary motion around a molecular axis has been controlled by electron transfer process and by photoexcitation. The basis of the motion is intramolecular rotation of a ligand (3,8-d-ethynyltrityl-1, 10-phenanthroline) around a copper axle. The asymmetric copper system is synthesized by immobilizing a "stator" to a silicon support. The "rotator," 3,8-di-ethynyltrityl-1, 10-phenanthroline is complexed to the metal center, Cu (I) or Cu (II) serving as an "axle". The Cu (I) system structure is tetrahedral, but that of Cu (II) is square planar. The interconversion of the two provides the basis for controlled, rotational motion. Hysteresis is observed in the different region of the applied voltage for different stators. The peak of the bis-P-Si shifts to the left compared to that of the phen-Si stator because of the larger energy gap of phen-Si. The energy states of the Cu (I) and Cu (II) are extracted from the transport measurement results.

11:51AM Q24.00004 Simultaneous Measurements of Force and Conductance through Single Molecular Junctions, MICHAEL FREI, Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York, MARIA KAMENETSKA, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Labs, Upton, New York, LATHA VENKATARAMA-MAN — We measure the conductance of single molecules attached to gold electrodes by repeatedly forming and breaking junctions between a gold substrate and a gold-coated cantilever in a modified atomic force microscope (AFM). While transport through single molecular junctions has been investigated, we gain additional information through the simultaneous recording of the forces required to break these junctions. Specifically, the force traces show elastic and plastic deformation processes hidden in conductance measurements. Our single molecular conductance measurements reproduce the results obtained previously and we find that the forces required to break gold point-contacts is consistent with published results. Furthermore, we present a comparison of measured forces required to break the Au-N bond formed in our single molecule junctions and densities functional theory (DFT) results.

12:03PM Q24.00005 Dielectrophoretic Trapping of Au Nanoparticles using High Quality Nanogap Electrodes, YE LU, DANVERS E. JOHNSTON, DOUGLAS R. STRACHAN, BETH S. GUITON, PETER K. DAVIES, TAE-HONG PARK, MICHAEL J. THERIEN, A. T. CHARLIE JOHNSON, University of Pennsylvania — In the past decade, single molecule-based electronic devices have drawn enormous attention. One of the great challenges to be overcome is the fabrication of well-defined, uncontaminated nanogap electrodes, and the subsequent assembly of individual molecules or nanoparticles onto the contacts. A promising route to this goal is the feedback controlled electromigration (FCE) drawn enormous attention. One of the great challenges to be overcome is the fabrication of well-defined, uncontaminated nanogap electrodes, and the subsequent assembly. Methods for controlling DEP assembly by modification of the electrostatic interaction between NPs and substrate surfaces are explored. Funding: NSF-NSEC/NBIC DMR-0425780. 1D. R. Strachan et al., Appl. Phys. Lett. 86 043109 (2005). 2D. R. Strachan et al., Nano. Lett. 86 043109 (2006).

12:15PM Q24.00006 Nanomechanical Shuttling of Electrons, E. M. WEIG, D. R. KOENIG, J. P. KOTTHAUS, Center for NanoScience & Department of Physics, Ludwig-Maximilians University Munich, Germany — A nanoscale metal island that is oscillating between two opposing electrodes on a vibrating string can be used to mechanically actuate an electric current. We have realized such an electron shuttle on a doubly clamped high Q silicon nitride beam subject to high tensile strain. The shuttle is operated acoustically which guarantees complete decoupling of the measured signal from the drive at arbitrary source drain voltages. We have investigated the shuttling current across the island as a function of the applied voltage bias under resonant actuation. Since the tunnel resistance increases exponentially with distance, charge transfer between the island and an electrode only occurs at the turning points of the shuttle motion. Therefore transport across the island is strictly sequential, so that the shuttle can be theoretically described using a single electron box model during contact time. We have observed excellent agreement between our measured data and theoretical calculations which suggests that a crossover to the Coulomb blockade regime should be observed for smaller sample dimensions and lower temperatures.

12:27PM Q24.00007 Measuring the momentum of a nanomechanical oscillator using tunnel junctions, CHARLES DOIRON, Universitaet Basel, BJOERN TRAUZETTEL, Universitaet Wuerzburg, CHRISTOPH BRUDER, Universitaet Basel — We present a way to measure the momentum $p$ of a nanomechanical oscillator. The momentum detector is based on two tunnel junctions in an Aharonov-Bohm-type setup, where one of the tunneling amplitudes depends on the motion of the oscillator and the other one does not. The coupling between the first tunnel junction and the oscillator is assumed to be linear in the position $x$ of the oscillator $t(x) = t_0 + t_1 x$. However, the presence of two junctions can make the equation of motion for the density matrix of the coupled (oscillator+tunnel junction) system show that in this case the finite-frequency current noise of the detector is proportional to the momentum spectrum of the oscillator.

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12:39PM Q24.00008 Vibronic enhancement of phonon heat conductance\(^1\). YOSHIHIRO ASAI, National Institute of Advanced Industrial Science and Technology (AIST), Japan — We have studied the electron transport and phonon heat transport through single molecular bridge-junctions in terms of a newly proposed self-consistent theory. Due to the inelastic coupling between electrons and phonons, the two transport properties are closely correlated, which are treated on an equal footing. By using the theory we have studied the two problems, i.e., (1) the non-equilibrium phonon effect on the electron transport and (2) the inelastic vibronic coupling effect on the phonon heat conductance. We have discussed dissipation processes of the inelastic energy accompanying the electronic conduction through the bridge-junction. Ref) Y. Asai, Phys. Rev. Lett. 93, 246102 (2004); 94, 099901(E) (2005). Y. Asai and H. Fukuyama, Phys. Rev. B 72, 085431 (2005). Y. Asai, submitted.

\(^1\)This work has been supported by CREST-JST.

12:51PM Q24.00009 Anisotropic Phonon Propagation in Nanoporous Alumina\(^1\). AKIHIRO SATO, Max Planck Institute for Polymer Research, GEORGE FYTAS, F.O.R.T.H Institute of Electronic Structure and Laser Technology, BAHRAM DJAFARI-ROUHANI, YAN PENNEC, Institut d’Electronique, de Micro-électronique et de Nanotechnologie, MARTIN STEINHART, Max Planck Institute of Microstructure Physics, WOLFGANG KNOLL, Max Planck Institute for Polymer Research — Self-ordered nanoporous alumina membranes contain highly ordered hexagonal arrays of cylindrical holes. Phononic crystals based on nanoporous alumina with various porosities represent a composite medium for rich elastic wave propagation phenomena due to their periodicity and acoustic impedance contrast between alumina and infiltrated materials. It allows the manipulation of the high frequency acoustics as probed by Brillouin light scattering. In-plane and out-of-plane (perpendicular to the holes) propagation of the elastic waves are distinctly different. While the former reveals an effective medium and localization behavior, the latter selects the medium filling the holes. Band structure theoretical calculations provide a semiquantitative description of the new experimental findings.

\(^1\)This study was partially supported by a grant-in-aid from Marubun Research Promotion Foundation.

1:03PM Q24.00010 Phononic Properties of Periodic 1D Multilayer Polymer Films, NIKOLAOS GOMOPOULOS, WEI CHENG, Max Planck Institute for Polymer Research, GEORGE FYTAS, F.O.R.T.H Institute of Electronic Structure and Laser Technology, TARAS GORISHNYY, EDWIN THOMAS, Massachusetts Institute of Technology, ANNE HILTNER, ERIC BAER, Case Western Reserve University — The evolution of phonon dispersion relation with composition and periodicity in 1D periodic multilayer nanoscale polymer films is studied using high resolution Brillouin light scattering. An increase in complexity of the dispersion relation as the lattice constant \(d\) becomes comparable to the phonon wavelength \((q \sim 1)\) is observed. Films with large \(d\) include phonons propagating within individual layers, as opposed to delocalized phonons moving throughout an effective homogeneous medium in films with small \(d\). Temperature dependent measurements of the sound velocities reveal the presence of distinct glass transition temperatures in support of the distinct propagation of phonons through the periodic medium in agreement with theoretical predictions. The structure related elastic excitations are determined by the product of the layer thickness and the phonon wave vector \(q\) and hence all layer guided modes are superimposed in a reduced plot of the phase velocity \(v\) vs \(q\).

1:15PM Q24.00011 Dephasing of the weak localization correction in networks of quantum dots\(^1\). JOERN N. KUPFERSCHMIDT, PIET W. BROUWER, LASSP, Cornell University — We consider the corrections to the conductance of networks of quantum dots due to electron-electron interactions. Interaction corrections are calculated to first order in the propagator associated with the capacitive coupling among the dots. We focus in particular on calculating the dephasing correction to the weak localization correction and the Altshuler-Aronov correction to the conductance.

\(^1\)Supported by the Cornell Center for Materials Research

1:27PM Q24.00012 Fractal conductance fluctuations of classical origin, HOLGER HENNIG, RAGNAR FLEISCHMANN, MPIDS, Goettingen and University of Goettingen, Germany, LARS HUFNAGEL, Kavli Institute for Theoretical Physics, UCSB, USA, THEO GEISEL, MPIDS, Goettingen and University of Goettingen, Germany — The coherent conductance through mesoscopic structures is well known to show reproducible fluctuations with the variation of an external parameter (e.g. a magnetic field). These fluctuations are caused by interference effects and can be described semiclassically. In systems with mixed (regular and chaotic) classical dynamics fractal conductance curves are found. Experiments that study the transition from coherent to chaotic transport showing a change of the fractal dimension with the coherence-length\(^2\) however, seemed to contradict the semiclassical theory of the fractal scaling. We show that there is no contradiction but that the classical dynamics itself already leads to fractal conductance curves\(^3\) explaining the experimental observations. Moreover, we predict fractal classical conductance fluctuations not only in systems with mixed phase space but in purely chaotic systems.


1:39PM Q24.00013 Electron Transport through Models for Small-World Nanomaterials\(^1\). LAZARUS SOLOMON, MARK NOVOTNY, Mississippi State University — We investigate the quantum transport of (spinless) electrons through simplified models related to small-world nanomaterials. We employ a tight-binding Hamiltonian, and obtain the transmission coefficient from a matrix solution of the associated time-independent Schrödinger Equation. The system studied corresponds to \(d = 1\) semi-infinite input and output leads, connected to a 'blob' of \(N\) atoms. We first present exact results for \(N\) inter-connected atoms, a fully-connected graph. The exact solution, for any \(N\), is given both for symmetric and non-symmetric connections between the 'blob' and the input/output. We then present numerical results obtained by removing some of the connections within the \(N\)-site 'blob', thereby approaching transport through a small-world nanomaterial [1-4].


\(^1\)Supported in part by NSF.
11:15AM Q25.00001 Structure and Assembly of Dense Solutions and Melts of Polymer Tethered Nanoparticles, ARTHI JAYARAMAN, KENNETH S. SCHWEIZER, University of Illinois, Urbana-Champaign — We generalize the microscopic Polymer Reference Interaction Site Model theory to study intermolecular pair correlation functions and collective structure factors of dense solutions and melts of polymer-tethered spherical nanoparticles. The complex interplay of entropy (translational, conformational and packing) and enthalpy (particle-particle attraction) leads to different structural arrangements with distinctive scattering signatures. Strong concentration fluctuations indicative of aggregate formation and/or a tendency for microphase separation occur as the total packing fraction and/or particle-particle attraction strength increase. A microphase spinodal curve is estimated by extrapolation of the inverse of the amplitude of the small angle scattering peak. For nanoparticles, twice the diameter of monomers, carrying a single tether the microphase spinodal temperature grows roughly as a power law function of packing fraction with an exponent much less than unity. Increasing the nanoparticle diameter lowers the microphase spinodal temperature and results in a qualitative change of its packing fraction dependence. The effect of nanoparticle size, number and length of tethers, position of the grafting sites, total packing fraction, and particle-particle attraction strength on the structure, scattering patterns and tendency for microphase ordering has been studied in detail.

11:27AM Q25.00002 Line shape analysis of dynamic light scattering results on polymeric microgel nanoparticles, KIRIL A STRELETZKY, IMAAN BENMERZOUGA, JOHN MCKENNA, Cleveland State University — Hydroxypropylcellulose (HPC) is nontoxic polysaccharide with temperature dependent water solubility. HPC polymer chains can be chemically cross linked into stable nanoparticles—microgels. HPC microgel properties depend on polymer and salt concentration and cross linking density. One of the most important properties of HPC is its critical temperature of 41°C, at which the polymer undergoes a reversible phase transition. HPC microgels also undergo a reversible volume phase transition in which particles shrink considerably. This property might lead to application of microgels as effective targeted drug delivery and release system. We used Dynamic Light Scattering to study microgels at different temperatures and applied line shape analysis algorithm to analyze resulting spectra. We found that the microgel initial size depends heavily on polymer concentration. We also found that varying salt concentration affects the dynamics of microgels. In addition, we were able to determine the effective cross linking density that yields relatively monodisperse microgels. We explored the structure of several microgel solutions by angular dependence analysis and found that most of them were spherical particles. In addition, we explored dynamics of the same microgels at different temperatures that enabled us to monitor their shrinking behavior.

11:39AM Q25.00003 Neutron Flow-Mapping of Controlled-Architecture Polymer Melts, TOM MCLEISH, Dept of Physics and Astronomy and Polymer IRC, Univ. of Leeds, NIGEL CLARKE, Dept of Chem./Polymer IRC, Univ. of Durham, PIERRE CHAMBON, Dept of Chem./Polymer IRC, Univ. of Sheffield, EDOARDO DE LUCA, Dept of Chem./Polymer IRC, Univ. of Durham, JOHN EMBERY, Dept of Physics and Astronomy and Polymer IRC, Univ. of Leeds, CHRISTINE FERNYHOUGH, Dept of Chem./Polymer IRC, Univ. of Sheffield, TIM GOUGH, Dept of Mech. Eng.,/ Polymer IRC, Univ. of Bradford, RICHARD GRAHAM, School of Mathematical Sciences, Univ. of Nottingham, ISABELLE GRUJO, Institut Laue-Langevin, France, LIAN HUTCHINGS, Dept of Chem./Polymer IRC, Univ. of Durham, KAMAKSHI JAGANNATHAN, HARLEY KLEIN, Dept of Physics and Astronomy and Polymer IRC, Univ. of Leeds — We report on results of a new method for probing complex flows of entangled polymer melts that is able to compare simultaneously chain configurations on different length scales and stress distribution in the flow with the predictions of molecular models. Controlled-architecture melts synthesised by anionic polymerisation and selectively deuterated are made in sufficient quantities to fill a recirculating flow device. The whole processing rig is scanned across a narrow neutron beam. The motion is then detected by measuring the induced e.m.f in the electrode. As a first step in understanding possible damping effects due to metal films, we have fabricated free standing metallic resonators. We have fabricated doubly clamped beams out of Al, Au, and Au/Pd alloys (dimensions length 3−5µm, thickness ≈ 100 nm, width 200 nm). Beams of this dimension have a resonant frequency around 5−10 MHz. We will report measurements, performed in a dilution refrigerator, of the quality factor Q in these resonators as a function of temperature and magnetic field (up to 15 T).

11:51AM Q25.00004 Chain dynamics in a semifluoropolymer solution under steady shear, PRASANTH JOSE, GRZEGORZ SZAMEL, Department of Chemistry, Colorado State University, Fort Collins, CO 80523 — We performed a series of Brownian dynamics simulations of sheared semifluoropolymer solutions of relatively short polymer chains and found that incomplete cancellation of intra and inter chain contributions to the steady state structure factors leads to anisotropic patterns that resemble those observed in light scattering experiments on sheared semifluoropolymer solutions (J. Chem. Phys. 122, 114905(2007)). Here we investigate the changes in the single-chain dynamics in sheared semifluoropolymer solutions. We study the shear-rate dependence of the end-to-end vector relaxation, Rouse modes' dynamics, etc. We correlate the changes in the chain dynamics with shear rate dependence of the anisotropic scattering patterns and shear thinning of the solution viscosity.
12:03PM Q25.00005 Investigation of Extensional Flow-induced Crystallization in Entangled Polymer Melts. JONG KAHK KEUM, YIMIN MAO, FENG ZUO, BENJAMIN S. HSIAO, Stony Brook University. TEAM — To investigate the extensional flow-induced crystallization of semidilute and concentrated polymer solutions, synchrotron X-rays have been used. The results show that the formation of crystallization precursor structure (i.e., shish-kebab structure) under extensional flow is strongly governed by applied strain as well as strain rate. A critical strain rate exists in the formation of flow-induced crystallization precursor structure. Below this critical strain rate, no shish-kebab structure can be formed even when the applied strain is higher than the critical strain rate. Results confirmed that the crystalline shish precursor structure is formed first and it induces the growth of folded-chain lamellae, i.e., kebabs.

12:15PM Q25.00006 Transport and rheology in block copolymer mesophases. XUSHENG ZHANG, JORGE VINALS, McGill University — Free energy functionals of an order parameter field are widely used to describe ordered phases and flows in block copolymer melts. We present a systematic derivation of the transport equations governing order parameter diffusion and hydrodynamic flows by considering the order parameter and the local deformation as the two independent variables. By studying the static and dynamic response of the copolymer, we derive expressions for the reactive and dissipative components of the stresses. We finally use these equations to study the low frequency rheology of the copolymer under an applied oscillatory shear.

12:27PM Q25.00007 Universal Scaling of Linear and Nonlinear Rheological Properties of Semidilute and Concentrated Polymer Solutions. RONALD LARSON, YOUNGSUK HEO, University of Michigan — We examine the validity of the de Gennes “blob” concept in predicting linear and nonlinear rheological properties of semidilute polystyrene solutions in tricresyl phosphate (TCP). At a fixed value of reduced concentration c/ce where ce is the entanglement concentration, below a critical value of around 2.0 for our polystyrene/TCP solutions, linear and nonlinear rheological functions superimpose after the modulus and the frequency (or shear rate) of each solution are respectively normalized with the concentration-dependent plateau modulus and the equilibration time obtained from the de Gennes scaling relationships using the literature value of the solvent-quality exponent 0.53. However, once the polymer volume fraction exceeds the “swelling volume fraction” above which the polymer takes on a random walk configuration on all length scales even in a good solvent, this universal scaling breaks down and the polymer conformation appears to be governed by Colby-Rubinstein’s scaling laws for theta solutions. We estimate that all polybutadiene solutions in phenyl octane (a good solvent) from the work of Colby et al. are above the swelling concentration and can be scaled using theta solvent scaling laws for concentrations ranging all the way up to the melt, showing universal behavior of melts and solutions above the swelling concentration.

12:39PM Q25.00008 The linear rheological responses of cyclic polyoctenamer melt. MIAO HU, GREGORY MCKENNA, Department of Chemical Engineering, Texas Tech University, YAN XIA, ROBERT GRUBBS, JULIE KORNFIELD, Division of Chemistry and Chemical Engineering, California Institute of Technology. — There is continuing interest in the dynamics of macrocyclic polymers or polymer rings. Here we are working with novel polyoctenamer rings synthesized by a ring opening metathesis polymerization (ROMP) route that precludes linear contamination when pure catalyst is used. While the rings are polydisperse in their molecular weights, the method permits synthesis of extremely high molecular weight entities. Here we report results on the dynamic moduli and the zero shear rate viscosities of both the cyclic polyoctenamer of Mw up to nearly 400,000 g/mol (which is nearly 50 entanglements) and the linear analogue. Comparisons will be made with prior literature results on rings made by ring closure methods in dilute solution where contamination with linear chains was problematic and where the entanglement density was less than 20.

12:51PM Q25.00009 Rheology and birefringence of Fomblin YR at very high shear rates. KHALED MRIZIQ, HANK COCHRAN, MARK DADMUN, University of Tennessee. — Simultaneous measurements of the rheological and structural properties of perfluoropolyether (PFPE) lubricant films were measured at relatively low to extremely high shear rates using a rotational optical rheometer. The viscosity of various films with different thicknesses exhibit Newtonian behavior up to a shear rate 1x10^4 s^-1, with a transition to shear-thinning behavior obvious at higher shear rates. Birefringence of these films was also measured, and these results indicate chain alignment with shear in the shear-thinning regime. The shear rate at which alignment occurs is similar to that of the onset of shear thinning. This correlation between chain alignment and shear thinning provides direct evidence that the ability of PFPEs to lubricate hard drives at high shear rates is a direct consequence of the ability of the applied shear field to align the molecules on a molecular level.

1:03PM Q25.00010 Rheo-Dielectric Studies of Concentrated Polysisoprene Solutions. JAI PATHAK, RICCARDO CASALINI, C. M. ROLAND, NRL, Chemistry, SIMONE CAPACCIOLI, University of Pisa, Physics, NIKOS HADJICHRISTIDIS, University of Athens, Chemistry. — We have performed dielectric spectroscopy on concentrated and well-entangled cis-1,4-polysoprene solutions in n-tetradecane while they undergo steady shear. The volume fraction of polymer is 0.2, and the number of entanglements per chain varies between 20 and 30. cis-1,4-Polysoprene is a Stockmayer Type-A dipole, with one dipole moment component along the chain backbone. Hence dielectric spectroscopy on it reveals the global chain relaxation (normal mode), in addition to its segmental mode relaxation. We critically examine the normal mode in strongly non-linear flows in the cone (22.8 mm diameter)-platen (25 mm) geometry. We work with a sea of fluid surrounding the cone, and the edge remains intact deeper into the shear thinning regime. In addition to visual inspection of the sample edge, we also check for validity of the Cox-Merz rule, finding good agreement between the two. Preliminary results indicate that the dielectric strength continually decreases well into the non-linear regime, perhaps a consequence of the orthogonal directions of the dielectric measurement (velocity gradient direction) and the chain stretching (flow direction).

1:15PM Q25.00011 Isothermal and Self-Seeding Crystallization from Polyethylene Solution. HOWARD WANG, NARAYAN CH DAS, KAIKUN YANG, Department of Mechanical Engineering and Institute of Materials Research, Binghamton University, SUNY, Binghamton, NY 13902, BOUALEM HAMMOUDA, National Institute of Standards and Technology, Gaithersburg, MD 20899. — We have applied time-resolved small angle neutron scattering (SANS) to studying self-seeding and isothermal crystallization kinetics of low molecular weight polyethylene in solution. In one example, SANS spectra of isothermal crystallization of 2.1 kg/mol PE at 78.8 °C from a solution containing 4.3% PE by mass show both the characteristic form and structure factors of stacked lamellae. The intensity hump around 0.025 Å^-1 indicates the correlation among lamellae. On the other hand, SANS from the same solution after quenched from melt to the room temperature, then stored at 90 °C for 5 min, followed by quenching to 78.7 °C are different from those of isothermal crystallization; the first correlation peak from the structure factor is not obvious, implying that crystals are dominantly in single or few lamellae forms. A morphological model that accommodates arbitrary distributions of structures from individual lamellae to infinite stacks has been used to analyze the SANS data. A possible lyotropic transition from isolated to stacked lamellae is suggested.

1This work is supported by the National Science Foundation.
1:27PM Q25.00012 Retention behavior of star-shaped polymers near the chromatographic critical condition. JESSE ZIEBARTH, YONGMEI WANG, University of Memphis, KYUHYUN IM, HAE-WOONG PARK, YOUNGTAK KIM, SUNYOUNG AHN, TAIHYUN CHANG, Pohang University of Science and Technology — The retention behavior of star-shaped polymers near the liquid chromatographic critical condition (LCCC) was investigated with 2-D liquid chromatography of polystyrene (PS) and lattice Monte Carlo simulations. At the LCCC for linear PS, stars with short arms elute after linear PS, while stars with long arms show a cross-over from late to early elution as branch number increases. Monte Carlo simulations show that two factors, excluded volume interactions and attractive end-effects resulting from initiator butyl groups, are required to explain the elution of star polymers. When polymers are modeled by random walk chains without excluded volume interactions, all stars are slightly more attracted to pores than corresponding linear chains. When polymers are modeled as self-avoiding walks (SAW) that include excluded volume interactions, stars with short arms elute later and stars with long arms elute earlier compared to linear chains. Incorporating more attractive-ends in SAWs results in more attractive to pores than corresponding linear chains. More attractive ends in PS star samples were confirmed through chromatographic retention of stars with short arms elute later and stars with long arms elute earlier compared to linear chains. In addition, no significant dependence of the hole burning event on entanglement density was observed.

1:39PM Q25.00013 Mechanical Hole Burning Spectroscopic Investigation. QIAN QIN, GREGORY MCKENNA, Texas Tech University — Mechanical spectral hole burning (MSHB) was previously applied to a densely entangled block copolymer and successfully distinguishes the heterogeneous from the homogeneous state. Here, we chose polystyrene (PS) solutions to further investigate the effect of entanglement density on mechanical spectral hole burning. The entanglement density was varied by changing either solution concentration or molecular weight of the PS. Dynamics in different regimes ranging from close to the Rouse regime into the terminal region were also examined. Our results are consistent with a heterogeneous dynamics over both entanglement (or plateau) and Rouse regimes. Terminal relaxation dynamics, on the other hand, were always found to be homogeneous for the PS/diethyl phthalate solutions investigated. In addition, no significant dependence of the hole burning event on entanglement density was observed.

1:51PM Q25.00014 Linking number of linear chain in polymer solution and melts. QI LIAO, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100080, China — We present the statistical results of linking number of linear chains prepared by Monte Carlo and molecular dynamics simulations of polymer solution and melts. Simulations were performed for a wide range of chain lengths covering both non-entangled and entangled polymer dynamics. The simulation results for linking number dependence on chain length and distribution function are compared with the prediction and conjecture of topology.

2:03PM Q25.00015 Computer simulation study on the shear-induced phase separation in semidilute polymer solutions by using Ianniruberto-Marrucci model. SHOTARO NISHITSUJI, MIKHITOK TAKENAKA, Graduate School of Engineering, Kyoto University, TAKASHI TANIGUCHI, Graduate School of Science and Engineering, Yamagata University, HIROKAZU HASEGAWA, Graduate School of Engineering, Kyoto University — When shear flow is imposed to a semi-dilute polymer solution at its one phase region, the solution exhibits strong turbidity. This phenomenon is called shear-induced concentration fluctuation and/or phase separation. Theoretically, Doi and Onuki submitted a two fluid model which incorporates the gradient term of the stress tensor into Ginzburg-Landau type free energy functional, and account for the spatial heterogeneity of the stress field by dynamic asymmetry. We developed the new computer simulation scheme with Doi-Onuki theory, where the Ianniruberto-Marrucci model (IM model) is employed as the constitutive equation, to simulate the dynamics of the shear-induced concentration fluctuation and/or phase separation in semi-dilute polymer solutions. In the simulation results, the concentration fluctuations appear and coarsen with time under shear flow and the change in shear stress with time exhibits the overshoot behavior due to the relaxation of entanglement. These results agree with the experimental results.

Wednesday, March 12, 2008 11:15AM - 2:15PM – Session Q26 DCP: Advances in Spectroscopy Morial Convention Center 218

11:15AM Q26.00001 IR and Raman spectroscopy of water and ice by ab initio simulations1. MANU SHARMA, DAVIDE DONADIO, GIULIA GALLI, UC Davis — We use ab initio molecular dynamics to compute the IR and Raman spectra of a variety of heavy water systems, ranging from pure water and ice, to liquid water confined between graphene foils and D-terminated diamond surfaces. The analysis of the simulated spectra provides the fingerprints of different hydrogen bonding environments, giving access to the complex structural and dynamical properties of water in various conditions. In addition our results provide a detailed, microscopic interpretation of IR and Raman experiments, as they allow us to assign univocally spectroscopic bands to specific vibrational modes, and to identify electro-dynamic coupling between water molecules and surfaces, in the case of confined water. Our MD simulations also give a quantitative assessment of the anharmonicities and lifetimes of various vibrational modes.

1This work was performed under the auspices of the DOE under contract no. W-7405-Eng-48

11:27AM Q26.00002 Infrared spectra of ice and water from first principles: intra vs. intermolecular dipole correlations1. WEI CHEN, Department of Physics, Princeton University, Princeton, NJ 08544, USA, MANU SHARMA, Department of Chemistry, University of California, Davis, CA 95616, USA, RAFFAELE RESTA, Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, 34014 Trieste, Italy, GIULIA GALLI, Department of Chemistry, University of California, Davis, CA 95616, USA, ROBERTO CAR, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — We report simulated infrared (IR) spectra of deuterated ice and water using Car-Parrinello molecular dynamics with maximally localized Wannier functions. Experimental features of both ice and water are accurately reproduced within the harmonic approximation. Calculated line shapes are further decomposed in terms of intra and intermolecular dipole correlation functions with spatial resolution. This approach proves to be very useful to understand the origin of spectral features and the nature of the underlying hydrogen-bond (H-bond) network. We find that intermolecular dynamic charge fluctuations play a crucial role over the entire frequency range.

1This work is partially supported by NSF under the PCCM-MRSEC program with award number: NSF DMR 02-13706.
11:39 AM Q26.00003 Nuclear quantum effects in water. JOSEPH MORRONE, ROBERTO CAR, Dept. of Chemistry, Princeton University — In this work, a path integral Car-Parrinello molecular dynamics simulation of liquid water is performed. It is found that the inclusion of nuclear quantum effects systematically improves the agreement of first-principles simulations of liquid water with experiment. In addition, the proton momentum distribution is computed utilizing a recently developed “open” path integral molecular dynamics methodology. It is shown that these results, which are consistent with our computations of the liquid structure, are in good agreement with neutron Compton scattering data. The remaining discrepancies between the present results and experimental data are indicative of some degree of over-binding in the hydrogen bond network, likely engendered by the use of semi-local approximations to density functional theory in order to describe the electronic structure.

1 This work was supported by the Fannie and John Hertz Foundation and DOE grant DE-FG02-05ER46201

11:51 AM Q26.00004 ABSTRACT WITHDRAWN

12:03 PM Q26.00005 Fluorescence correlation spectroscopy with Gaussian-Lorentzian volumes. MICHELE MARROCCO, ENEA — Fluorescence correlation spectroscopy (FCS) is a fundamental technique of fluorescence microscopy used for many applications of chemical physics where molecular diffusion plays primary roles [see, for example, O. Krichhevsky and G. Bonnet, Rep. Prog. Phys. 65, 251 (2002)]. The milestone of FCS is called three-dimensional Gaussian (3DG) approximation. According to this assumption, the observation volume is modeled by Gaussian profiles along the main three spatial directions. This simplification is necessary to achieve analytical treatment of FCS measurements. In this work, analytical solutions are shown for another geometry corresponding to the fundamental mode of laser beams, i.e. the Gaussian-Lorentzian distribution, where Gaussian profiles are associated with the two transverse directions while a Lorentzian dependence characterizes the axial direction (coincident with the optical axis of the microscope). Analytical solutions are guaranteed only for both one-photon and two-photon excitations of diffusing molecules [one-photon excitation is considered in M. Marocco, Chem. Phys. Lett. 449, 227 (2007)]. Similarities and differences with respect to the 3DG approximation are discussed.

12:15 PM Q26.00006 Studying hydrogen bond by Quantum Monte Carlo: binding energy and dispersion curve of the water dimer. LEONARDO SPANU, SISSA-ISAS Trieste, Italy; Dept. of Chemistry UC Davis, FABIO STERPONE, LUCA FERRARO, Caspur Roma, Italy, SANDRO SORELLA, SISSA-ISAS Trieste, Italy, LEONARDO GUIDONI, Univ. La Sapienza Roma, Italy — We present a variational MonteCarlo (VMC) and lattice regularized diffusion MonteCarlo (LRDMC) study of the binding energy and dispersion curve of the water dimer. One the aim of the present work is to investigate how the bonding of two water molecules, as a prototype of the hydrogen-bonded complexes, could be described by a JAGP wave function, an implementation of the resonating valence bond idea. Using a Pseudopotential for the inert core of the Oxygen, with a full optimization of the variational parameters, we obtain at the VMC level a binding energy of -4.5(0.1) Kcal/mol, while LRDMC gives -4.9(0.1)Kcal/mol (exp. 5 Kcal/Mol). The calculated dispersion curve reproduces both at the VMC and LRDMC level the minimum position and the right curvature. The quality of the WF gives us the possibility to dissect the binding energy in different contributions by appropriately switching off determinantal and Jastrow terms in the JAGP: we estimate the dynamical contribution to the binding energy of the order of 1.4(0.2) Kcal/Mol whereas the covalent one about 1.0(0.2) Kcal/Mol. JAGP reveals thus a promising WF for describing systems where dispersive and covalent forces play an important role.

12:27 PM Q26.00007 Hydrogen bond network ordering of liquid water confined between two metallic plates studied by ab initio molecular dynamics. MARIVI FERNANDEZ-SERRA, Physics & Astronomy SUNY Stony Brook — We present an ab initio molecular dynamics study of liquid water confined between two palladium (111) surface slabs, at room temperature. We analyze in detail the layering and ice-Ih-type ordering of water molecules close to the metal interfaces. In particular we show how water molecules next to the metal surface display a very different structural and dynamic behavior as compared to those in the “bulk” regions, which can be easily characterized using infra-red spectroscopy. Hydrogen bonds near the metallic surfaces are strengthened, inducing a characteristic ordering which decays with de distance from the surfaces. Our preliminary results show that this confined water presents an asymmetrical and stable structure as a function of Z (axis perpendicular to the surfaces) which results in a characteristic ordering of the water molecules resembling that of ferroelectric systems.

12:39 PM Q26.00008 Quasiparticle lifetime and edge localized states of graphite studied by high-resolution ARPES. KATSUAKI SUGAWARA, TAKAFUMI SATO, SEIGO SOUMA, TAKASHI TAKAHASHI, Tohoku University, HIROHITO SUEMATSU, RIKEN, Spring-8 — We have performed an ultrahigh-resolution angle-resolved photoemission spectroscopy (ARPES) of high-quality graphite single crystal (kish graphite) to elucidate the band structure and many-body interaction. We clearly observed an extremely small hole-like Fermi surface centered at the K(H) point, a sharp quasiparticle peak in the vicinity of the Fermi level ($E_F$), and a kink in the dispersion at 0.18 eV. 1 We also found first evidence for the edge localized states near $E_F$, whose energy dispersion is markedly different from that of the bulk band. We will discuss the energy- and temperature-dependence of quasiparticle lifetime in relation to the strong electron-phonon coupling, the electron-plasmon interaction, and the electron-hole pair excitations. 2 K. Sugawara et. al., Phys. Rev. Lett. 98 (2007) 036801. 2 K. Sugawara et. al., Phys. Rev. B 73 (2006) 045124.

12:51 PM Q26.00009 Fully ab-initio study of the optical response of charged rare gas clusters. FERNANDO NOGUEIRA, Center for Computational Physics and Physics Department, University of Coimbra, Portugal, MICAELE OLIVEIRA, Center for Computational Physics, University of Coimbra, Portugal and European Theoretical Spectroscopy Facility, MIGUEL MARQUES, LPMCN, Universitè Lyon 1, Lyon, France and European Theoretical Spectroscopy Facility — Charged rare-gas clusters are markedly different from their neutral, van der Waals bonded counterparts. The removal of an electron from a strongly antibonding orbital causes the bonding to become much stronger and shifts the optical absorption to the visible region. We report a fully ab-initio determination of the geometry, electronic structure, and optical response of small singly charged Ne, Ar, Kr and Xe clusters. All calculations were performed using a pseudopotential based real space implementation of Time-Dependent Density-Functional Theory. We find that GGA leads, in general, to much better results than LDA, even though it predicts some absorption peaks at slightly higher energies than those found experimentally. The lighter elements show a single absorption peak but in the heavier elements spin-orbit interaction induces a splitting of the absorption peak, in good agreement with experiment.

1 This work was supported by Fundação para a Ciência e Tecnologia through grants #POCI/FIS/58309/2004 and #SFRH/BD/12712/2003.
the correlation length and the actual distance between two defects, the lattice spacing and the domain-wall size. Ad hoc directions and the crystal axes break the site-by-site translational invariance along the chain. Both these phenomena affect slow relaxation. We will show how...
11:27AM Q27.00002 Dynamical correlations of spin-1/2 chains . RODRIGO PEREIRA, University of British Columbia, STEVEN WHITE, UC Irvine, IAN AFFLECK, University of British Columbia — We show that the long-time behavior of the self-correlation function \( \langle S_i^z(t) S_j^z(0) \rangle \) of the S=1/2 XXZ model in the critical regime is dominated by high-energy excitations. We relate the exponents of the long-time decay to phase shifts which are known exactly from the Bethe ansatz. The same exponents are connected with the singularities of the dynamical structure factor \( S^{zz}(q, \omega) \). By combining the analytical results with the time-dependent density matrix renormalization group (tDMRG), we calculate \( S^{zz}(q, \omega) \) to very high precision.

11:39AM Q27.00003 Finite-temperature lineshapes in gapped quantum spin chains . ROBERT KONIK, Brookhaven National Laboratory, FABIAN ESSLER, University of Oxford — We consider the finite-temperature dynamical structure factor (DSF) of gapped quantum spin chains such as the spin one Heisenberg model and the transverse field Ising model in the disordered phase. At zero temperature the DSF in these models is dominated by a delta-function line arising from the coherent propagation of single particle modes. Using methods of integrable quantum field theory we determine the evolution of the lineshape at low temperatures. We show that the line shape is in general asymmetric in energy and becomes Lorentzian only at temperatures far below the gap. We discuss the relevance of our results for the analysis of inelastic neutron scattering experiments on gapped spin chain systems such as CsNiCl₃ and YBaNiO₅.

11:51AM Q27.00009 Magnetic field versus temperature phase diagram of the spin-1/2 bond-alternating-chain antiferromagnet \( F_{2}PNN \). YASUO YOSHIDA, Kyushu University; University of Florida, TATSUYA KAWAI, Kyushu University, BOHDAN ANDRAKA, YASUMASA TAKANO, University of Florida, YUKO HOSOKOSHI, Osaka Prefecture University, KATSUYA INOUE, Hiroshima University, NOBUYA MAESUMA, Tohoku University, Institute for Molecualr Science, KOUICHI OKUNISHI, Kanazawa University, KYOMI OKAMOTO, Tokyo Institute of Technology, TORU SAKAI, Japan Atomic Energy Agency — The S = 1/2 Heisenberg bond-alternating-chain antiferromagnet pentfluorophenyl nitronyl nitroxide (\( F_{2}PNN \)) exhibits Tomonaga-Luttinger-liquid behavior in the temperature dependence of the specific heat above the field-induced magnetic ordering temperature [1]. We have determined the magnetic phase diagram of this compound from the specific heat. For a single crystal, the boundary of the ordered phase in the field-versus-temperature diagram is symmetric with respect to the central field of the gapless region \( H_{c1} \leq H \leq H_{c2} \), whereas a distorted phase boundary is observed for a powder sample, whose ordering temperature is reduced. Calculations based on the finite-temperature density-matrix renormalization group suggest the possibility of a novel incommensurate phase due to frustration in the powder, in a narrow field range near the central field. [1] Y. Yoshida et al., Phys. Rev. Lett. 94, 037203 (2005).

12:03PM Q27.00005 Correlation amplitude and entanglement entropy in random spin chains¹ . JOSÉ HOYOS, Duke University, ANDRÉ VIEIRA, Universidade Federal do Ceará, NICOLAS LAFLORENCIE, CNRS-Orsay, EDUARDO MIRANDA, Universidade Estadual de Campinas — Using strong-disorder renormalization group, numerical exact diagonalization, and quantum Monte Carlo methods, we revisit the random antiferromagnetic XXZ spin-1/2 chain focusing on the long-length and ground-state behavior of the average time-independent spin-spin correlation function \( C(t) = \langle S_i(t) S_j(0) \rangle \). In addition to the well-known universal (disorder-independent) power-law exponent \( \eta = 2 \), we find interesting universal features displayed by the prefactor \( v = v_{l}/s \), if \( l \) is odd, and \( v = v_{o}/s \), otherwise. Although \( v_{l} \) and \( v_{o} \) are nonuniversal (disorder dependent) and distinct in magnitude, the combination \( v_{l} + v_{o} = -1/4 \) is universal if \( C \) is computed along the symmetric (longitudinal) axis. The origin of the nonuniversalities of the prefactors is discussed in the renormalization-group framework where a solvable toy model is considered. Moreover, we relate the average correlation function with the average entanglement entropy, whose amplitude has been recently shown to be universal. The nonuniversalities of the prefactors are shown to contribute only to surface terms of the entropy. Finally, we discuss the experimental relevance of our results by computing the structure factor whose scaling properties, interestingly, depend on the correlation prefactors.

¹ Supported by NSF, Research Corporation, FAPESP, CNPQ, NSERC, and ManNEP

12:15PM Q27.00006 Electronic and magnetic properties of the chain compounds K₃T₂O₄ (T=Ni, Pd, Pt) . KLAUS KOEPERNIK, IFW, Dresden, DEEPA KASINATHAN, WALTER SCHNELLE, HELGES ROSNER, MPI CPS, Dresden — Recent susceptibility measurements on the chain compound K₃Pd₂O₄ were interpreted in terms of localized spin 1/2 Pd moments on one of the two crystallographically different Pd sites, only [R. V. Pasin et al., J. Solid St. Chem. 180, 1566 (2007)]. The main exchange interaction was reported to be antiferromagnetic from the negative Curie-Weiss temperature \( \theta = -80K \). Earlier measurements for the isostructural and isovalent Ni and Pt compounds suggest an antiferromagnetic coupling for T=Ni as well as ferromagnetic for T=Pt. [H. Zentgraf et al., Z. Anorg. allg. Chem., 462, 92 (1980)] Here, we report an electronic structure study focusing on the interplay of covalency, spin-orbit coupling and correlation to describe the behavior of this compound family. The inclusion of strong Coulomb repulsion at the transition-metal sites is necessary to obtain the correct insulating ground state observed in recent measurements for the Pd system. The origin of the different magnetic behavior will be discussed.

12:27PM Q27.00007 ABSTRACT WITHDRAWN –

12:39PM Q27.00008 muSR study on quasi-one-dimensional cobalt/rhodium oxides . PETER RUSSO, TRIUMF, JUN SUGIYAMA, H. NOZAKI, Y. IKEO, K. MUKAI, Toyota CRDL, T. TAKAMI, University of Texas at Austin, H. IKUTA, DANIEL ANDREICA, ALEX AMATO, LMU-PSI — Thanks to the unique power of muon spin spectroscopy, we found that the quasi-one-dimensional Co-Rh oxides \( A_{n+2}CoRh_{n}O_{3n+3} \) \((A = Ca, Sr; n=1, 2, 3)\) exhibit a two-dimensional antiferromagnetic transition that ranges from approximately 185 K for \( n=1 \) to 125 K for \( n=3 \) with a transition width \( (\Delta T) \) of about 80 K. The variation of \( T_{N}^{c} \) with \( n \) is explained by the increase in the distance between the neighboring CoRh \( O_{3n+3} \) chains. Static magnetic order is observed below the endpoint of \( N = (T_{N}^{c} - \Delta T) \) for each of the three compounds. The existence of the two-frequency components in the ZF-spectrum indicates the appearance of ferrimagnetic order for \( A_{3}CoRhO_{6} \) below 20 K.
1:03PM Q27.00010 $^{51}$V NMR Study of a quasi-1D XXZ spin chain system BaCo$_2$V$_3$O$_8$, K.-Y. CHOI, NHMFL, FSU, Tallahassee, FL32306-4390, USA, N.S. DALAL, REYES COLLABORATION, P.L. KUHNS COLLABORATION, H.D. ZHOU COLLABORATION, C.R. WIEBE COLLABORATION — We present $^{51}$V NMR measurements on the quasi-one-dimensional $S=1/2$ XXZ antiferromagnet BaCo$_2$V$_3$O$_8$ along the chain. The $^{51}$V NMR spectrum shows that the quantum phase transition takes place from the Néel ordered phase to the incommensurately ordered phase around $T_C = 4$ T. In addition, we studied a spin-lattice relaxation rate, $1/T_1$, as a function of temperature and field. Our results are compared to a theoretical prediction and are discussed in terms of a softening of spinons in an external field.

1:15PM Q27.00011 Spin Supersolid in Anisotropic Spin-One Heisenberg Chain, PINAKI SENGUPTA, CRISTIAN BATISTA, LANL — We consider an $S = 1$ Heisenberg chain with strong exchange ($\Delta = J_s/J_1$) and single-ion uniaxial anisotropy ($D$) in a magnetic field ($B$) along the symmetry axis. The low energy spectrum is described by an effective $S = 1/2$ XXZ model that acts on two different low energy sectors for a finite range of fields. The vacuum of each sector exhibits Ising-like antiferro magnetic ordering coexisting with the finite spin stiffness obtained from the exact solution of the XXZ model. In this way, we demonstrate the existence of a spin supersolid phase. We also compute the full $\Delta - B$ quantum phase diagram using a quantum Monte Carlo (QMC) method.

1:27PM Q27.00012 Interacting vs. free quasi-particle description for the spin-1/2 chain, SEBASTIAN EGGER, MICHAEL BORTZ, University Kaiserslautern, MICHAEL KARBACH, University Wuppertal, IMKE SCHNEIDER, University Kaiserslautern — We consider the individual excitations of the antiferromagnetic spin-1/2 chain in the Luttinger Liquid formalism. The inclusion of Umklapp scattering and other irrelevant operators introduces an interaction between quasi-particles, which lifts the degeneracy in the linearized spectrum. So far this effect has been systematically understood only for the lowest excited state in each sector. We now show for a number of low lying excitations how rotations in the degenerate subspaces diagonalize the Umklapp term perturbatively. Our results are verified by taking advantage of the Bethe solution of the spin chain to perform an exact finite size scaling analysis for individual excited levels. From this we can identify the correspondence of quantum numbers between the bosonic and Bethe states. We also make contact to the well known quantum numbers at the non-interacting free fermion point.

1:39PM Q27.00013 Magnetic Susceptibilities of Finite Ising Chains in the Presence of Defect Sites, SERGEI GOUPALOV, University of Utah & Ioffe Institute, DANIEL MATTIS, University of Utah — Any antiferromagnet with zero net magnetic moment exhibits limited response to an external homogeneous magnetic field. This changes dramatically in the presence of defect sites, even those that carry no spin. We examine the excess susceptibilities, longitudinal and transverse, due to one or more defects at arbitrary separations in a finite Ising chain with nearest-neighbor couplings. Adapting matrix methods to finite chains we derive exact formulas valid at all $T \geq 0$.

1:51PM Q27.00014 Excitation spectrum and magnetic properties of the new Haldane-gap material NENB, SERGEI ZVYAGIN, Dresden High Magnetic Field Laboratory (HLD)/Research Center Dresden - Rossendorf (FZD), E. ČIŽMÁR, M. OZEROV, O. IGNATCHIK, T. PAPAGEORGIOU, J. WOSNITZA, NHMFL/Florida State University, Z. ZHOU, Wayne State University, J.L. WIKAIRA, University of Canterbury, C.P. LANDEE, M.M. THURNBULL, Clark University — Results of high-field ESR and magnetization studies of the new spin-1 Haldane-chain material $[Ni(C_{12}H_{12}N_2)_2NO_3(BF_4)]$ (NENB) are reported. A definite signature of the Haldane state in NENB was obtained. From the analysis of the frequency-field dependence of magnetic excitations in NENB, the spin-Hamiltonian parameters were calculated, yielding $\Delta/k_B = 17.4$ K, $\delta || = 2.14$, $D/k_B = 7.5$ K, and $E/k_B = 0.7$ K for the Haldane gap, $\delta$ factor and the crystal-field anisotropy constants, respectively. The presence of fractional $S = 1/2$ chain-end states, revealed by ESR and magnetization measurements, is found to be responsible for spin-glass freezing effects. In addition, extra states in the excitation spectrum of NENB have been observed in the vicinity of the Haldane gap, which origin is discussed.

2:03PM Q27.00015 Direct comparison of hole doping effects due to cation and to oxygen content on magnetic properties of the spin-chain system $Ca_{3+y}Y_{2-}^{+}Cu_{O_{10-}^{−}y}$, KEESEONG PARK, THEODORE CACKOWSKI, JOHN MARKERT, Department of Physics, The University of Texas at Austin — A quasi-one dimensional system, $Ca_{3+y}Y_{2-}^{+}Cu_{O_{10-}^{−}y}$ (CaY-CuO) is studied to compare the magnetic effects of cation doping with those of oxygen deficiency. Hole doping ($p$) due to cation concentration ($x$) and oxygen deficiency ($\delta$) in other copper oxides is often observed to obey $p = x - 2\delta$. CaYCuO has a simple edge shared CuO$_2$ structure and is hole dopable up to a formal copper valence of 2.4. Various Ca doped CaYCuO specimens were fabricated in different oxygen environments, including high pressure oxygen up to 170 atm. X-ray diffraction and iodometric titration were used to confirm phase and oxygen content. Samples are found to be more oxygen deficient with increasing cation doping. Magnetic moment and specific heat were measured. The antiferromagnetic phase was observed up to $x = 1.0$ doping for fully oxygenated specimens. Néel temperatures decreased with increasing cation doping and decreasing oxygen deficiency. The decrease in Néel temperature is found to be more than expected from hole doping $p = x - 2\delta$. A new quantity that describes all of the behavior of Néel temperature, $x = (2/3)\delta$, is proposed.

2:15PM Q28.00001 Thermoelectric Transport Coefficients in Correlated Condensed Matter, SRIRAM SHASTRY, University of California Santa Cruz — We present a recently developed formalism for computing thermoelectric transport coefficients for standard models of correlated matter, such as the Hubbard and the $t-J$ model. Successful predictions of this method in the context of the Hall constant are noted. This success helps to motivate the extension to the Seebeck coefficient, the Lorenz number $L$, and the figure of merit $ZT$. In terms of novel equal time correlation functions of two new fundamental operators, the thermal operator $\Phi^{xx}$ and the thermoelectric operator $\Phi^{xz}$. Along the way, we uncover a new sum rule for the dynamical thermal conductivity for many standard models, precisely analogous to the f-sum rule for the electrical conductivity. Also along the way, we throw light on Lord Kelvin's early ideas on reciprocity, worked out within the context of equilibrium thermodynamics. The precise connection between Kelvin's formulation, and the later and more rigorous formulation of Onsager is commented upon. The new formalism is tested in simple settings and recent computational results are displayed for testing the frequency dependence of these variables in certain standard models. Close agreement with existing transport experiments on sodium cobaltates Na$_{0.68}$CoO$_2$ in the Curie Weiss phase is found. Finally some new predictions are made regarding triangular lattice systems, motivated by the sodium cobaltate system.

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$^{1}$Supported by grants NSF-DMR-0706128, and DOE-BES DE-FG02-06ER46319

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q28 DMP FIAP: Focus Session: Thermoelectricity in Bulk Materials

11:15AM Q28.00001 Thermoelectric Transport Coefficients in Correlated Condensed Matter

1Supported in part by grants NSF-DMR-0706128, and DOE-BES DE-FG02-06ER46319
11:51 AM Q28.00002 Enhancing figure-of-merit of n-type Bi$_2$Te$_3$-$x$Sb$_x$. XIAO YAN, JIAN YANG, YI MA, BED POUEL, YUCHENG LAN, DEZHI WANG, ZHIFENG REN, QING HAO, GENG CHEN, MIT COLLABORATION — Thermoelectric materials with high dimensionless figure-of-merit (ZT) are greatly demanded in energy industry, among which bismuth telluride (Bi$_2$Te$_3$) exhibits decent ZT around room temperature. However, thermal conductivity of Bi$_2$Te$_3$ is still high which limits its wider use for low temperature cooling devices. Here we investigate nanostructured bulk n-type Bi$_2$Te$_3$-$x$Sb$_x$ by reducing the thermal conductivity via increased phonon scattering of the significantly increased grain boundaries due to nano size grains. We first made alloy nanocrystals by mechanical alloying a mixture of elements with the right ratio and then 100% nanostructured samples by hot press.

12:03PM Q28.00003 High pressure transport studies on Sb$_2$Te$_3$ and BiSbTe$_2$. MATTHEW JACOBSEN, ANDREW CORNELIUS, University of Nevada, Las Vegas — Interest regarding the abilities of thermoelectric materials has produced exciting results regarding their properties in the thin-film form [3]. However, little work has been done regarding the pressure tuning of the thermoelectric figure of merit for these materials. Some previous work has suggested that it would be useful to investigate this further using pressure tuning [1,2]. Based upon this interest, facilities have been developed in our laboratory for the study of the relevant properties under high pressure up to near 20 GPa. Results of this work on Sb$_2$Te$_3$ and BiSbTe$_2$ will be presented here from the use of these facilities. [1]Gény, G., Dresselhaus, M.S., Dresselhaus, G., Fleurial, J.-P., and Caillat, T. Recent developments in thermoelectric materials. International Materials Reviews, 48, 45-66 (2003). [2]Rowe, D.M. CRC Handbook of Thermoelectric Materials. CRC Press, 1995. [3]Venkataramanan, R., Silvola, E., Colpitts, T., and O’Quinn, B. Thin film thermoelectric devices with high room-temperature figures of merit. Nature, 413, 597-602, 2001.

12:06PM Q28.00004 Inelastic scattering on antimony bearing thermoelectric materials: rattlers revisited. R. P. HERMANN1, W. SCHWEIKA, Institut fuer Festkoerperforschung - Forschungszentrum Juelich, Germany, H.-C. WILLE2, ESRF, Grenoble, France — Antimony element specific measurements on EuFe$_2$Sb$_12$ and Zn$_2$Sb$_3$ will be presented in parallel with inelastic neutron scattering measurements on Zn$_2$Sb$_3$. These results yield new insight in the rattler concept. First, the antimony specific DOS in EuFe$_2$Sb$_12$ and Co$_2$Sb$_3$ provides experimental insight into the guest-host interaction mechanism which is required for a lowering of the thermal conductivity[1]. Second, the scattering vector dependence of the Zn$_2$Sb$_3$ inelastic response reveals that “rattling” behavior is not restricted to single atoms and that more complex structural units, such as dumbbells, can exhibit a similar behavior that is responsible for a low thermal conductivity.[2] The European Synchrotron Radiation Facility is acknowledged for provision of the synchrotron radiation facility at beamlines ID18 and ID22N and the European Community - ARI HPR-2001-00175 is acknowledged for provision of neutron scattering beam time at the FR-J-II research reactor in Juelich, Germany. [1] Schwei W. et al. Phys. Rev. Lett. 99, 125501 (2007). [2] Wille H.-C. et al. Phys. Rev. B 76, 140301(R) (2007).

12:27PM Q28.00005 ABSTRACT WITHDRAWN –

12:39PM Q28.00006 Lattice thermal conductivity of AgSbTe$_2$. DONALD MORELLI, Michigan State University, VLADIMIR JOVOVIC, SURAJ THIAGARAJAN, JOSEPH HEREMANS, The Ohio State University — The lattice thermal conductivity of high-quality crystals of AgSbTe$_2$ is nearly temperature-independent from 80 to 300 K, and has a value of 0.65±0.05 W/mK. This value corresponds to the minimum possible thermal conductivity, where the phonon mean free path equals the interatomic distance. The result is analyzed in terms of scattering mechanisms: Umklapp and Normal phonon-phonon scattering processes are the dominant mechanism. It is, to our knowledge, the first system in which intrinsic phonon-phonon interactions limit the lattice thermal conductivity to such a low value. This in turn results from the extreme anharmonicity of the chemical bonding in AgSbTe$_2$, which gives rise to one of the highest Gruneisen parameter of any solid. The phonon-phonon scattering rate being a function of the square of the latter, the lattice thermal conductivity is also one of the lowest.

12:51PM Q28.00007 Galvanomagnetic and thermomagnetic properties of AgSbTe$_2$. VLADIMIR JOVOVIC, JOSEPH HEREMANS, The Ohio State University — We report here data on the electrical resistivity, magnetoresistance, Hall effect, thermoelectric power, magneto-Seebeck and transverse Nernst-Ettingshausen coefficients of high-quality crystals of AgSbTe$_2$, measured from 77 to 400 K in magnetic fields up to 2 Tesla. Thermal conductivity data are also reported in samples with a much higher carrier concentration than those used in our other work. From an analysis of these data, we conclude AgSbTe$_2$ to be a very narrow-gap semiconductor (Eg≈ 7.6±3 meV) with ~5x10$^{19}$ cm$^{-3}$ holes in a valence band with a high density of states and thermally excited ~10$^{17}$ cm$^{-3}$ high-mobility (2.200 cm$^2$/Vs) electrons at 300 K. The estimated hole density-of-states effective masses, including Fermi pocket degeneracy, is 2.5±0.5 free electron masses; the electron mass is about two orders of magnitude smaller, but the exact value cannot be resolved. The lattice term dominates the thermal conductivity, and the electronic contribution in samples with both electrons and holes present is in turn dominated the ambipolar term. The low thermal conductivity and very large hole mass of AgSbTe$_2$ make it a most promising p-type thermoelectric material.

12:51PM Q28.00008 De Haas - van Alphen quantum oscillations in AgSbTe$_2$. JOSEPH HEREMANS, VLADIMIR JOVOVIC, The Ohio State University — Quantum oscillations are observed in the magnetic susceptibility of p-type single crystals of AgSbTe$_2$, at 5 K in magnetic fields up to 5 Tesla (the De Haas - van Alphen effect). The period of the oscillations is analyzed in terms of the cross-section of the hole Fermi surface. Recent band structure calculations illustrate the dependence of the hole Fermi surface structure on the ordering of the Ag and the Sb atoms on the metal sublattice, and provide guidance for the interpretation of the periods of the oscillations. Galvanomagnetic studies of the same sample provide a hole density of 5x10$^{19}$ cm$^{-3}$, so that an image for the valence band Fermi surface can be Reconstructed at that carrier density level. The measured Fermi surface cross-sections, together with the transport properties, give an overall picture that is consistent with the calculation valid for AgSbTe$_2$, with Ag and Sb ordered on the metal sublattice. [1] Khang Hoang, S. D. Mahanti, James R. Salvador, and Mercouri G. Kanatzidis, Atomic Ordering and Gap Formation in AgSb-Based Ternary Chalcogenides, Phys. Rev. Lett. 2007, accepted [2] V. Jovovic and J. P. Heremans, Galvanomagnetic and Thermomagnetic properties of AgSbTe$_2$, abstract here.

1This work is supported by BSST-Amerigon.
1:15PM Q28.00009 Precipitation anneals in the PbTe-PbS system\textsuperscript{1}. CHRISTOPHER JAWORSKI, VLADIMIR JOVOVIC, JOSEPH HEREMANS, The Ohio State University — Bulk samples of (PbS)\textsubscript{x}(PbTe)\textsubscript{1-x} have been prepared in the range 4\% < \< 15\%. There is a miscibility gap in the pseudo-binary PbTe/PbS phase diagram that enables the precipitation of a PbS-rich phase in a PbTe-rich matrix. To that effect, the samples were compounded in the liquidus, and then quenched, resulting in a supersaturated solution. Conditions for precipitation anneals were then developed, and samples with nano-precipitates of a PbS-rich phase in a PbTe-rich parent phase have been obtained, as evidenced by X-ray diffractions. This technique, previously applied to Pb-rich PbTe\textsuperscript{1}, is aimed at creating a bulk material containing a substantial fraction of nanometer-sized particles in order to mimic the morphology of quantum-dot superlattices that reached very high values of the thermoelectric figure of merit. Preliminary thermoelectric and thermal conductivity data will be presented, along with galvanomagnetic and thermomagnetic data aimed at identifying the electronic properties of the materials. [1] J. P. Heremans, C. M. Thrush and D. T. Morelli, Thermopower enhancement in PbTe with Pb precipitates, J. Appl. Phys. 98 063703 (2005) [2] T. C. Harman, M. P. Walsh, B. E. LaForge, and G. W. Turner, J. Electron. Mater. 34, L19 (2005).

\textsuperscript{1}This work is supported by BSST-Amerigon.

1:27PM Q28.00010 High-Resolution \textsuperscript{125}Te NMR of Novel Thermoelectric Materials, E.M. LEVIN, K. SCHMIDT-ROHR, B.A. COOK, Ames Laboratory DOE and Iowa State University, MI-KYUNG HAN, M.G. KANATZIDIS, Northwestern University — Several novel Te-based thermoelectric materials with extraordinary figure of merit ZT > 1.4 have been studied by high-resolution 25 kHz magic angle spinning \textsuperscript{125}Te nuclear magnetic resonance (NMR) in order to investigate variations in composition on the nano-scale. A 20-fold wider \textsuperscript{125}Te NMR signal of both AgSbGe\textsubscript{2}Te\textsubscript{5} and AgSbGe\textsubscript{5}Te\textsubscript{7} (\textgreek{g}= -90 kHz) compared to that of PbTe (4.5 kHz) indicates a variation of shifts due to local composition fluctuations. The similar total shift of the main peak in Ag\textsubscript{0.53}Pb\textsubscript{1.5}Sb\textsubscript{1.2}Te\textsubscript{20} (-1790 ppm) and PbTe (-1750 ppm) and similarly long T\textsubscript{2} relaxation time show that the majority of Te atoms in both materials has a similar environment. A second peak in Ag\textsubscript{0.53}Pb\textsubscript{1.5}Sb\textsubscript{1.2}Te\textsubscript{20} at -1600 ppm shows the presence of a second type of Te site, accounting for \textgreek{g}/3 of all Te. These are apparently located in (Ag, Sb)-rich inclusions, as indicated by a much shorter T\textsubscript{2}, which can be due to the effect of quadrupolar relaxation of \textsuperscript{125}Sb or \textsuperscript{125}Te (spin 5/2 or 7/2, respectively) on \textsuperscript{125}Te. Our data confirm suggestions made by Hsu et al., Science (2004) and by Chen et al., Appl. Phys. Lett. (2005) about the presence of nano-scale inclusions in Ag\textsubscript{0.53}Pb\textsubscript{1.5}Sb\textsubscript{1.2}Te\textsubscript{20}, which result in low lattice thermal conductivity and high ZT.

1:39PM Q28.00011 Substitution effects on the thermoelectric properties of Sr\textsubscript{3}IrO\textsubscript{4}, YANNICK KLEIN, ICHIRO TERASAKI, Waseda University, Tokyo — Layered cobalt oxides with the low-spin (LS) state, such as Na\textsubscript{2}CoO\textsubscript{2} and Ca\textsubscript{2}CoO\textsubscript{4}, have shown a good potential as p-type materials for thermoelectric applications [1, 2]. Layered rhodium oxides are also characterized by a high Seebeck coefficient and a low metallic resistivity [3, 4]. The LS configuration of the transition metal is considered to be at the origin of this unusual property. We have investigated the thermoelectric properties of Sr\textsubscript{3}IrO\textsubscript{4}, which is isostructural to the superconductors La\textsubscript{2}CuO\textsubscript{4} and Sr\textsubscript{2}RuO\textsubscript{4}. Contrary to the later ones, Sr\textsubscript{3}IrO\textsubscript{4} is a semiconductor with a narrow gap and a weak ferromagnetic ground state (T\textsubscript{c} \approx 240K, M\textsubscript{S} \approx 0.14\textmu B/\textmu m) [5]. For polycrystalline samples, the resistivity is of the order of 10\textsuperscript{11} cm and the thermoelectric power shows a broad maximum around 110K (S \approx 300\textmu V/K\textsuperscript{-1}) denoting the activation of minority carriers. In order to increase the carrier concentration, we tried many substitutions for Sr and Ir. Results of resistivity, thermoelectric power and susceptibility will be discussed.


1:51PM Q28.00012 Temperature - Concentration Phase Diagram from First Principles Calculations in P\textsubscript{2}-Na\textsubscript{2}CoO\textsubscript{4}\textsuperscript{1}. YING S. MENG, University of Florida, YOYO HINUMA, GERBRAND CEDER, Massachusetts Institute of Technology — The unusual electronic and magnetic properties of Na\textsubscript{2}CoO\textsubscript{4} are attracting considerable interest in recent years. At high sodium content, the system displays unusually strong thermoelectric effect and a low metallic effect. In this paper, we present temperature - concentration phase diagram for Na\textsubscript{2}CoO\textsubscript{4} (0 < x < \approx 0.5) obtained with first principles method of the Density Functional Theory (DFT) in the Generalized Gradient Approximation (GGA) scheme, where charge on Co is delocalized. In comparison we will also present the results obtained from the GGA with Hubbard U correction (GGA+U) scheme, where charge on Co is localized.

\textsuperscript{1}US Department of Energy under Contract No. DE-FG02-96ER-45571

2:03PM Q28.00013 ABSTRACT WITHDRAWN —


11:15AM Q29.00001 Quantized transport in graphene p-n junctions, CHARLES MARCUS, Harvard University — No abstract available.

11:51AM Q29.00002 Local-Gating of Graphene Nanostructures, JAMES WILLIAMS, CHARLES MARCUS, Harvard University — We report on the fabrication and measurement of locally-gated single-layer graphene devices. Utilizing a non-covalent functionalization layer, the preservation of the unique electrical properties of graphene after deposition of the top-gate oxide is demonstrated. Novel top-gate geometries, including circular and multiple-rectangular gate designs, combined with oxygen-plasma etching allow for further elucidation of the unique transport properties of graphene p-n junctions and graphene constrictions. Research supported in part by INDEX, an NRI Center, and by the Harvard NSEC.
12:03PM Q29.00003 Scanning tunneling microscopy and spectroscopy of graphene.1, GUOHONG LI, ADINA LUCIAN, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — We report low temperature high magnetic field scanning tunneling microscopy and spectroscopy on a graphene sheet suspended above a graphite substrate by extended defects. The measurements provide the first observation of the V-shaped density of states in zero field and of the Landau level (LL) spectrum in finite fields. The LL spectrum consists of a single sequence exhibiting square root dependence on field and level-index, and contains a zero energy LL attributing to the chiral nature of the Dirac Fermi quasiparticles. The density of states reflects important effects due to electron-phonon interactions and to confinement. These include a reduced Fermi velocity, a small (10 meV) gap at the Dirac point, splitting of the n=0 LL at relatively low fields and a new negative energy state that emerges from the Fermi level and splits away linearly with increasing field.

1Work supported by DOE DE-FG02-99ER45472 and NSF-DMR-0456473.

12:15PM Q29.00004 Electronic properties of one-dimensional graphene bilayer ribbons1, BHA-GAWAN SAHU, Microelectronics Research Center, University of Austin, Austin TX 78758, HONGKI MIN, ALLAN MACDONALD, Department of Physics, University of Texas, Austin TX 78712, SANJAY BANERJEE, Microelectronics Research Center, University of Texas at Austin, Austin, TX 78758 — The electronic properties of armchair and zigzag bilayer graphene nanoribbons are studied using ab-initio density functional theory. We study the effect of width and the electric fields (up to the dielectric breakdown field of SiO2) on their energy gaps [Sahu 2007]. We find metallic and semiconductor arm-chair ribbons and electric field has the effect of increasing the gap in metallic ribbons. The zigzag ribbons due to the edge magnetism show opposite behavior: gap decreases with increase in the applied electric field. We studied small ribbons (below 1 nm) as well as large ribbons (5 nm). In small width arm-chair semiconductor ribbons, the gap decreases whereas in large width ribbons, the gap increases with applied electric field. Sahu B, Min H, MacDonald AH, and Banerjee SK “Electronic properties of one-dimensional graphene bilayer ribbons” (Submitted to Physical Review B).

1Work supported by NRI-SWAN Center

12:27PM Q29.00005 Strong Coulomb interactions and weak disorder in graphene , MATTHEW FOSTER, IGOR ALEINER, Columbia University — We analyze the instabilities and compute the transport properties of the low-temperature conducting phase of graphene, using a renormalization group (RG) approach that incorporates both Coulomb electron-electron interaction and weak quenched disorder effects. Strong Coulomb interactions are treated within the large-N expansion. Using a perturbative renormalization group (RG) approach to study the effects of virtual processes, we find that at successively lower energy scales, for moderate to strong Coulomb interaction strengths, a type of non-Abelian vector potential disorder always asserts itself as the dominant elastic scattering mechanism for generic short-ranged microscopic defect distributions. Vector potential disorder appears in graphene due to, e.g., elastic lattice deformations (“ripples”). We combine the RG results with a quantum kinetic equation analysis of real processes, i.e. inelastic electron-electron scattering, which allows us to compute the temperature- and chemical potential-dependence of electronic and thermal transport coefficients due to elastic and inelastic scattering processes in various coupling regimes.

12:39PM Q29.00006 Electric Field Effect in Epitaxial Graphene Devices, XUEBIN LI, XIAOSONG WU, MICHAEL SPRINKLE, FAN MING, CLAIRE BERGER, RAGHUNATH MURALI, FARHANA ZAMAN, JAMES MEINDL, WALTER DE HEER, Georgia Institute of Technology — The electric field effect has been observed on epitaxial graphene multilayers grown on SiC substrates by thermal decomposition of SiC. Carriers mobilities up to 2.5×10^6cm^2/Vs have been measured. Both side-gated and top-gated graphene field effect transistors (FETs) have been fabricated using standard semiconductor processes on both the Si and the C face of the SiC substrates. In side-gated FETs, the gates are located on both sides of narrow graphene ribbons; source-drain resistance is measured by a gate bias of several volts. For top-gated FETs the resistance swing reaches a factor of 25. At the gate voltage corresponding to the maximum source-drain resistance, the Hall voltage changes sign indicating a transition from hole- to electron-carried transport, consistent with the graphene band structure. These results indicate the potential of epitaxial graphene as a platform for large-scale graphene based electronics.

12:51PM Q29.00007 Free-Standing 2-D Graphene Carbon Nanostructures, BRIAN HOLLOWAY, RONALD QUINLAN, Luna Innovations Incorporated, KUN HOU, College of William and Mary — Carbon nanosheets – a new, free-standing, two-dimensional carbon nanostructure – have been deposited on a metal, semiconductor, and insulating substrates by RF PECVD. Raman, SEM, TEM, SAED, XPS, AES, FTIR, and XRD all indicate that nanosheets are graphite sheets up to 8 µm in height and ≤1 nm in edge thickness. The nanosheets stand off the growth substrate in a manner similar to aligned nanotubes grown by CVD. In contrast to nanotubes, nanosheets do not require catalyst for growth and can be patterned after deposition using standard lithographic techniques. Hydrogen etching promotes the formation of the atomically thin structures while the anisotropic dipole created in the graphene planes by the plasma sheath promotes the vertical orientation. Due to their uniform height and the large number of edge emission sites, nanosheets have proven to be excellent field emitters. Nanosheet samples have produced up to 33 mA of current (32 mm^2 sample area); similar nanosheet samples have sustained 1.3 mA of current over 200 hours of testing with no degradation.

1:03PM Q29.00008 Superconducting Proximity Effect in Graphite Films, MASAHIKO HAYASHI, Akita University, HIDEO YOSHIOKA, Nara Women’s University, AKINOBU KANDA, University of Tsukuba — Theoretical analysis of superconducting current in graphite films (or graphen)in proximity to superconductors is presented. In this work, the band structure of the graphite film is treated seriously: because of the delicate band structure of graphite, the actual band structure of the film, which undergoes the effects of various external factors such as leads and gates, can show a wide variety. We introduce following three models: 1) graphen-like Fermi points, 2) semi-metal, 3) electron (or hole) pockets, and 4) semiconducting gap. The superconducting critical current Lc = \exp[-L/\xi(T)] is studied where L is the distance between two leads and \xi(T) is the coherence length in the graphite film. The temperature dependence of \xi(T) is largely affected by the band structure and by examining this dependence the electronic properties of the graphite film can be estimated. The results are compared with actual experiments.

1:15PM Q29.00009 Superconducting proximity effect in thin graphite films , A. KANDA, T. SATO, S. TANAKA, H. GOTO, Y. OOTUKA, Inst. Phys. and TIMS, Univ. Tsukuba and JST-CREST, K. TSUKAGOSHI, RIKEN, AIST, and JST-CREST, H. MIYAZAKI, RIKEN and JST-CREST, S. ODAA, Y. AOYAGI, RIKEN, Tokyo Inst. Tech. and JST-CREST — Gate-controlled superconducting proximity effect in thin graphite films is reported. A graphite film with thickness of 4 - 10 nm is connected to two aluminum superconducting electrodes, forming a SNS junction, and gate electric field is applied using a back gate. The critical supercurrent displays an ambipolar behavior, and for a fixed normal-state resistance the electron critical supercurrent with positive gate voltage is always larger than the hole critical supercurrent with negative gate voltage (electron-hole symmetry breaking). This effect is also observed in the critical temperature where the junction resistance vanishes. Furthermore, the critical supercurrent is proportional to \exp(-(T/Tc)^2), which has never been observed in other SNS systems. The details of the experimental results as well as their possible origins will be discussed.

1:27PM Q29.00010 Supercurrent in Graphene Josephson Transistors, WENZHONG BAO, UC-Riverside, FENG MIAO, GANG LIU, CHUNNING LAU — We investigate electrical transport in single or bi-layer graphene devices coupled to superconducting electrodes. In these two-dimensional Josephson junctions, we observed gate tunable supercurrent, multiple Andreev reflections and hysteretic current-voltage characteristics. Latest experimental progress on dependence of supercurrent on temperature, number of layers and source-drain separation will be discussed.
1:39PM Q29.00011 Conductance behaviors of point-contact graphene junctions with normal metal and superconducting tips\(^1\), W. K. PARK, S. WOLIN, C. CHIALVO, N. MASON, L. H. GREENE, Department of Physics and the Frederick Seitz Mater. Res. Lab., University of Illinois at Urbana-Champaign — The recent discovery of graphene, a truly two-dimensional carbon allotrope, has attracted great interest because of its novel physics and potential for new electronic device applications. Among a variety of theoretical predictions that await stringent experimental tests, reflectionless tunneling (Klein paradox) and specular Andreev reflection are most intriguing. Aiming at eventually probing such unique charge transport phenomena in graphene junctions, we first investigate conductance behaviors of the nanoscale graphene junctions made by point-contact techniques using simple metal (Au) and superconducting (Nb) tips. At low temperatures, the conductance data exhibit an inverse peak structure centered at zero bias, reminiscent of the theoretical density of states arising from the Dirac-like dispersion relation. Junctions with Nb show the additional superconducting gap feature. We will present sets of conductance spectra as a function of temperature, magnetic field, and gate voltage, and discuss possible mechanisms to explain the observed conductance behaviors.

\(^1\)Work supported by the U.S. DoE DEFG02-91ER45439 and by NSF-DMR-0706013 through the FSMLRL and the CMM at UIUC.

1:51PM Q29.00012 Josephson Current and Multiple Andreev Reflections in Graphene SNS Junctions\(^1\), IVAN SKACHKO, XU DU, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — The Josephson Effect and Superconducting Proximity Effect were observed in Superconductor-Graphene-Superconductor (SGS) Josephson junctions with coherence lengths comparable to the distance between the superconducting leads. By comparing the measured temperature and gate dependence of the supercurrent and the proximity induced sub-gap features (multiple Andreev reflections) to theoretical predictions, we find that the diffusive junction model yields close quantitative agreement with the results. This is consistent with the fact that the measured mean free paths in these junctions, 10 ~ 30 nm, are significantly shorter than the lead separation. We show that all SGS devices reported so far fall in the diffusive junction category.

\(^1\)Work supported by DOE DE-FG02-99ER45742, NSF-DMR-0456473 and ICAM.

2:03PM Q29.00013 Electric field effect modulation and hysteresis in thin graphite using ferroelectric gate oxides, X. HONG, K. ZOU, J. ZHU, Department of Physics, Penn State University, A. POSADAS, J. REINER, C. H. AHN, Department of Applied Physics, Yale University — We study the electronic properties of thin graphite field effect transistors (FETs) using ferroelectric gate oxide Pb (Zr,Ti)O\(_3\) (PZT). Thin graphite flakes (3-5nm) are exfoliated onto 300 nm PZT films epitaxially grown on doped SrTiO\(_3\) (STO) and fabricated into FET devices. Carriers are induced into the FETs by applying a voltage \(V_g\) on the STO substrate (backgate). We observe a maximum carrier density \((n)\) of \(\sim 4 \times 10^{13} \text{cm}^{-2}\) and a density modulation of \(\sim 2 \times 10^{12} \text{cm}^{-2}/\sqrt{V_g}\) (\(V_g\)).


11:15AM Q30.00001 Correlations in carbon nanotubes: A DMRG approach, ALEXANDER STRUCK, SEBASTIAN A. REYES, SEBASTIAN EGGERT, Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany — Single wall carbon nanotubes (SWCNT) are a paradigm for studying quasi-one-dimensional systems with strong correlations, both experimentally and theoretically. Considering the strong relevance of SWCNT, it is even more surprising that only few numerical calculations of correlation effects have been attempted. In this talk, we use the density-matrix renormalization group (DMRG) technique to treat a recently formulated one-dimensional tight-binding lattice model, which accounts for both the electron motions around the circumference and along the tube axis. We discuss the influence of interactions of variable strength and range on the electronic structure and the electron density and outline possible finite-size and boundary effects.

11:27AM Q30.00002 First-Principles Electronic Structure Calculations of \(\text{N}_2\text{H}_4\) Adsorbed on Single-Wall Carbon Nanotubes\(^1\), M. YU, W.Q. TIAN, C.S. JAYANTHI, S.Y. WU, University of Louisville — Recent experiments conducted by Desai et al.\(^1\) reveal that single-wall carbon nanotube (SWCNT) networks exposed to \(\text{N}_2\text{H}_4\) vapor at various pressures exhibit considerable drop in resistance with respect to the pristine sample. Experimental findings reveal: (i) n-type behavior for the adsorption of \(\text{N}_2\text{H}_4\)/SWCNT, and (ii) the binding of \(\text{N}_2\text{H}_4\) on SWCNT as chemisorption. In the present work, we have performed first-principles electronic structure calculations\(^2\) for the \(\text{N}_2\text{H}_4\) adsorbed on the (14, 0) SWCNT, where several orientations for the \(\text{N}_2\text{H}_4\) molecule were considered. Calculations for the combined system were performed using 3 unit cells with the DFT/GGA and ultra soft pseudo-potentials. Our calculations reveal: (i) the binding of \(\text{N}_2\text{H}_4\) on SWCNT as physisorption, and (ii) the electronic structure of SWCNT to be practically unaffected by the adsorption of \(\text{N}_2\text{H}_4\), suggesting that there will not be a dramatic drop in resistance for \(\text{N}_2\text{H}_4$/ SWCNT. This is in disagreement with the experimental findings. To further understand the experimental observations, we will discuss mechanisms that may alter the binding nature of \(\text{N}_2\text{H}_4\) on SWCNT.\(^1\) S. Desai, G. Sumanasekera, et al. (APS, March 2008).\(^2\) G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996).

\(^1\)This work is supported by the US Army (SMDC).

11:39AM Q30.00003 First-principles calculations of effects of metallic electrode contacts on transport properties of carbon nanotubes, NOBUHIKO KOBAYASHI, Institute of Applied Physics, University of Tsukuba, TAISUKE OZAKI, Research Center for Integrated Science, Japan Advanced Institute of Science and Technology, KENJI HIROSE, Nano-Electronics Research Laboratories, NEC Corporation — Recently, considerable effort has been devoted to developing carbon nanotube devices. One of the important issues in the developments of carbon nanotube devices is the control of contact effects of the electrodes. To detect electric signals through nanotubes, electrodes must be connected to the nanotubes. Contact with the electrodes sensitively influences their electronic structures and transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculations that include the effect of contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes. The electronic states are calculated using a numerical atomic orbital basis set in the framework of the density functional theory, and the conductance is calculated using the Green’s function method. We have analyzed transport properties of the size of carbon nanotubes bridged between metallic electrodes, and discuss the contact effect of the electrodes on the transport properties. We reveal their dependency on the length and the electrode materials.
11:51AM Q30.00004 Effect of Phase-Breaking Events on Electron Transport in Single-Wall Nanotubes. THUSHARI JAYASEKERA, PAVAN PILLALAMARRI, J.W. MINTMIRE, Department of Physics, Oklahoma State University, Stillwater, OK, VINCENT MEUNIER, Oak Ridge National Laboratory, Oak Ridge, TN — Existing ballistic models for electron transport in single wall nanotube systems will break down as the size of the device becomes longer than the phase coherence length of electrons in the system. V. Krstic, et al. observed experimentally that the current in a SWNT system can be modified by a combination of a coherent and a non-coherent part. We analyze this problem in detail following Buttiker’s dephasing model. We investigate the effect of phase-breaking events on the electron transport in two-terminal single wall carbon nanotube systems, and discuss about more possible applications.

1The work carried out at Oklahoma State University is supported by the Department of Energy (DE-FG02-07ER46362) and the work at ORNL is supported by the Division of Materials Sciences and Engineering U.S. Department of Energy (DEAC05-00OR2272).

12:03PM Q30.00005 Local Gating in Carbon Nanotubes. JOSEPH SULPIZIO, Department of Physics, Stanford University, CHARIS QUAY, Stanford University, DAVID GOLDBADER-GORDON, Department of Physics, Stanford University — Single Wall Carbon Nanotubes (SWNTs) exhibit a host of remarkable physical properties. Their unique electronic structure suggests that SWNTs are ideal for studying the rich physics of one-dimensional (1D) quantum systems. Local gating enables the creation of tunable structures where such phenomena can be experimentally studied. We have fabricated locally-gated SWNT devices and have performed low-temperature electronic transport measurements. We present our recent data and discuss the results in the context of 1D mesoscopic systems.

12:15PM Q30.00006 Distinguishing the mechanisms of transistor-like switching in single-walled carbon nanotubes (SWCNTs). STEVEN HUNT, BRETT GOLDSMITH, PHILIP G. COLLINS — One of four mechanisms usually dominates the conductance switching of SWCNTs in field effect transistor geometries. In semiconducting SWCNTs, both the bandstructure and the Schottky barriers present at the SWCNT-electrode interface are sensitive to local electric fields. Disorder, too, leads to field sensitivity through SWCNT-SWCNT junctions and SWCNT defect sites. These four mechanisms can be distinguished by scanning gate microscopy, in which the local gating characteristics of interfaces, defects, and pristine sidewall can each be independently measured. We will demonstrate this separation and, in particular, focus on the gate sensitivity of sidewall defects produced by point functionalization. Scanning gate microscopy of SWCNTs before and after chemical attack allows us to visualize the electronic contributions of localized disorder and rank its contribution to three-terminal device characteristics.

12:27PM Q30.00007 Probing Vapor Phase Analytes with Single Walled Carbon Nanotube Biopolymer Hybrid Devices. SAMUEL KHAMIS, University of Pennsylvania Dept. of Physics and Astronomy, MICHELLE CHEN, University of Pennsylvania Dept of Materials Science and Engineering, A.T. CHARLIE JOHNSON, University of Pennsylvania Dept. of Physics and Astronomy — Single-Walled Carbon Nanotubes (SWCNTs) have attracted enormous interest due to their excellent electronic properties. The integration of SWCNTs into technologically relevant architectures is limited by the processing techniques available to address numerous integration challenges such as selective placement, doping and separation by electronic type. This talk will focus on using chemical methods to address the separation challenge by selectively functionalizing the metallic SWCNTs to fabricate field-effect transistors consisting of multiple SWCNTs. The process begins with a large-scale, low-loss purification of SWCNTs using a density step-gradient to allow for characterization of SWCNTs in large quantities. Once the material is purified, functionalized diazonium salts are used to selectively react with the metallic SWCNTs. Multiple SWCNT devices are then prepared and result in dramatically improved switching behavior. Methods to exploit the selective functionalization as a means of physically separating the material will also be discussed.

12:39PM Q30.00008 Selective Chemical Functionalization for the Fabrication of Single-Walled Carbon Nanotube Devices. GEORGE TULEVSKI, ALI AFZALI, PHAEDON AVOURIS, JAMES HANNON, IBM T.J. Watson Research Center — Single-Walled Carbon Nanotubes (SWCNTs) have attracted enormous interest due to their excellent electronic properties. The integration of SWCNTs into technologically relevant architectures is limited by the processing techniques available to address numerous integration challenges such as selective placement, doping and separation by electronic type. This talk will focus on using chemical methods to address the separation challenge by selectively functionalizing the metallic SWCNTs to fabricate field-effect transistors consisting of multiple SWCNTs. The process begins with a large-scale, low-loss purification of SWCNTs using a density step-gradient to allow for characterization of SWCNTs in large quantities. Once the material is purified, functionalized diazonium salts are used to selectively react with the metallic SWCNTs. Multiple SWCNT devices are then prepared and result in dramatically improved switching behavior. Methods to exploit the selective functionalization as a means of physically separating the material will also be discussed.

12:51PM Q30.00009 Electric Field Modulation of Thermoelectric Transport in Carbon Nanotubes and Graphene in the Quantum Transport Limit. YURI M. ZUEV, Applied Physics Department, Columbia University, PHILIP KIM, Physics Department, Columbia University — Mesoscopic thermoelectric power (TEP) measurements of nanometer scaled graphitic systems such as single walled carbon nanotubes (SWNTs) and graphene are reported. Highly transparent electrical contact was made to SWNTs using Pd electrodes. TEP was measured in-situ using a microfabricated heater and thermometers. Electrical conduction and TEP were observed at low temperature where both quantities were modulated by the gate voltage. At low temperatures, coherent quantum electric transport was observed as the conductance displayed oscillatory Fabry-Perot type interference. Simultaneously measured TEP provided corresponding oscillatory features. Deviations of the low temperature TEP gate dependence from the semiclassical Mott relation allows us to gain insight into the quantum transport regime in this one dimensional conductor. We compare these results with Butler’s dephasing model. We investigate the effect of phase-breaking events on the electron transport in two-terminal single wall carbon nanotube systems, and discuss about more possible applications.

1Work Supported by JSTO of the DTRA and the Army Research Office (W911NF-06-1-0462)

1:03PM Q30.00010 Thermal Conductivity of Single-Wall and Multi-Wall Carbon Nanotubes. NIHAR PRADHAN, Physics Department, WPI, MA, USA, HUANAN DUAN, JIANYU LIANG, Mechanical Engineering Department, WPI, MA, USA, GERMANO IANNACCHIONE, Physics Department, WPI, MA, USA — One-dimensional materials, such as nanotubes, and their composites attract interest due to their potential use in applications as well as model systems for understanding low-dimensional physics. There is a need for detailed measurements of the specific heat \(c_p\) and thermal conductivity \(\kappa\) in order to guide theoretical efforts. This talk presents \(c_p\) and \(\kappa\) using an ac-calorimetric technique for single-wall (SW) and multi-wall (MW) carbon nanotubes (CNT) in a composite sample-cell arrangement. From 300 to 400 K, \(c_p\) exhibits a linear behavior for both nanotubes. However, \(\kappa\) for MWNT and SWCNT with the heat flow perpendicular to the nanotube long-axis is bulk-like in behavior until \(\approx 370\) K, thereafter decreasing with increasing temperature, indicating the onset of phonon-phonon scattering. For samples where the heat flow is parallel to the nanotube long-axis, \(\kappa\) for the MWNT sample is consistent with ballistic phonon transport.
1:15PM Q30.00011 Efficient excitation energy transfer in single-walled carbon nanotube/porphyrin complexes, JOHN P. CASEY, SERGEI M. BACHILO, R. BRUCE WEISMAN, Department of Chemistry, Rice University — A novel method for generating single-walled carbon nanotube (SWNT) excited states by energy transfer from porphyrin molecules is presented. Addition of SWNTs to a series of micelle suspended porphyrins results in efficient quenching of porphyrin fluorescence. Analysis of concentration-dependent porphyrin quenching reveals that intermolecular energy transfer is associated with complex formation. Two-dimensional excitation/emission spectroscopy demonstrates that photosensitization of porphyrin absorption bands results in characteristic near-IR SWNT photoluminescence. The porphyrin/SWNT hybrid displays significantly shifted absorption and emission transitions as a result of strong electronic coupling between these two pi-conjugated systems. These interactions allow controllable tuning of SWNT transition energies. Complexation of SWNTs with organic photosensitizing molecules provides uniform excitation of a wide range of nanotube species in polydisperse samples using a convenient single excitation wavelength.

1:27PM Q30.00012 Heat Treatments In Situ and Noise Reduction in Metallic Single-Walled Carbon Nanotubes (SWCNTs), ALEXANDER KANE, PHILIP COLLINS, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697-4576 — As fabricated, small diameter metallic SWCNTs have anomalously high contact resistances and noise amplitudes. High temperature treatments have been found to decrease both the resistance and noise through undetermined mechanisms. This work investigates this high temperature processing through in situ measurements in a UHV environment, focusing on small metallic SWCNTs contacted by Ti, Pt, or Pd electrodes. The role of the contact resistance and contaminants in the device fluctuations or noise is studied. The two mechanisms affect device noise differently, with the net effect that room temperature noise decreases can be more than proportional to resistance decreases. Annealing temperatures for ideal device performance are determined for all three contact metals.

1:39PM Q30.00013 Dependence of the Raman G’ band intensity on metallicity of single-wall carbon nanotubes, KI KANG KIM, Sungkyunkwan University, JIN SUNG PARK, Tohoku University, SUNG JIN KIM, HONG ZHANG GENG, Sungkyunkwan University, KAY HYE S. AN, Jeonju Machinery Research Center, CHEOL-MIN YANG, Sungkyunkwan University, KENTARO SATO, RICHIRO SAITO, Tohoku University, YOUNG HEE LEE, Sungkyunkwan University — We report the peculiar behavior of the G’-band Raman intensity, which is dependent on the metallicity of single-wall carbon nanotubes (SWCNTs). In the metallic SWCNTs, the G’-band intensity was enhanced relative to the G-band intensity, while the G’-band intensity was suppressed in the semiconducting SWCNTs. Resonance Raman spectroscopy (using laser energies of \( \nu_{\text{Laser}} = 2.41 \, \text{eV}, 1.96 \, \text{eV}, \) and \( 1.165 \, \text{eV} \)) showed these features on the metal-enriched and semiconducting-enriched SWCNTs samples that had been selectively separated while the G’-band intensity was suppressed in the semiconducting SWCNTs. The metallicity dependence was explained theoretically by calculating resonance Raman intensity within the extended tight-binding model. The calculated results confirm that the G’-band intensity of the metallic SWCNTs is stronger than that for the semiconducting SWCNTs because the electron-phonon matrix elements for the TO phonon at the K point is larger for metallic SWCNTs and the resonance window for \( \nu_{\text{Laser}} ^{2} \) is larger than that for \( \nu_{\text{Laser}} ^{2} \).

1:51PM Q30.00014 Stability of finite single-walled carbon nanotubes adsorbed on Si(001)\(^{1}\), WALTER ORELLANA, Facultad de Ciencias Fisicas, Universidad Andres Bello — The stability and bonding properties of capped single-walled carbon nanotubes (CNTs) adsorbed on the Si(001) surface are studied using ab initio methods. We report the peculiar behavior of the G’-band Raman intensity, which is dependent on the metallicity of single-wall carbon nanotubes (SWCNTs). In the metallic SWCNTs, the G’-band intensity was enhanced relative to the G-band intensity, while the G’-band intensity was suppressed in the semiconducting SWCNTs. Resonance Raman spectroscopy (using laser energies of \( \nu_{\text{Laser}} = 2.41 \, \text{eV}, 1.96 \, \text{eV}, \) and \( 1.165 \, \text{eV} \)) showed these features on the metal-enriched and semiconducting-enriched SWCNTs samples that had been selectively separated while the G’-band intensity was suppressed in the semiconducting SWCNTs. The metallicity dependence was explained theoretically by calculating resonance Raman intensity within the extended tight-binding model. The calculated results confirm that the G’-band intensity of the metallic SWCNTs is stronger than that for the semiconducting SWCNTs because the electron-phonon matrix elements for the TO phonon at the K point is larger for metallic SWCNTs and the resonance window for \( \nu_{\text{Laser}} ^{2} \) is larger than that for \( \nu_{\text{Laser}} ^{2} \).

\(^{1}\)Research supported by the FONDECYT grant 1050197 and the Anillo Project ACT/24 (Chile)

2:03PM Q30.00015 Brownian Dynamics Simulations of Single-Wall Carbon Nanotube (SWNT) Separation by Type using Dielectrophoresis, MANUEL J. MENDES, Applied Physics, NOE ALVAREZ, Dep. Chemistry, HOWARD SCHMIDT, R. Smalley Inst., MATTEO PASQUALI, Dep. Chemical and Biomolecular Eng., Rice Univ. — We theoretically investigate the separation of individual metallic and semiconducting SWNTs in a dielectrophoretic (DEP) flow device. The SWNTs motion is simulated by a Brownian Dynamics (BD) algorithm including the translational and rotational effects of hydrodynamic, Brownian, dielectrophoretic, and electrophoretic forces. The device geometry is chosen to be a coaxial cylinder, because it yields effective flow throughput, and all fields can be described analytically. We construct a flow-DEP phase map, showing different regimes depending on the relative magnitudes of the forces in play. The BD code is combined with an optimization algorithm that searches for the conditions which maximize the separation performance. The optimization results show that a 99% performance can be achieved with typical SWNT parameters by operating in a region of the phase map where metallic SWNTs orient with the electric field, whereas the semiconducting SWNTs flow align. We show spectroscopic measurements of experimental tests which demonstrate metallic vs. semiconductor separation at frequencies in the MHz range. These results reveal crucial knowledge on the influence of the surfactant on the SWNTs effective conductivity.

Wednesday, March 12, 2008 11:15AM - 2:15PM – Session Q31 DMP DCOMP: Computational Nanoscience: Nanotubes and Graphene

11:15AM Q31.00001 Possible Precursors for Boron Nanotubes: A Novel Bonding Picture in Boron Sheets and Nanotubes, HUI TANG, SOHRAB ISMAIL-BEIHI, Department of Applied Physics, Yale University — Boron nanotubes (BNTs) have attracted a great deal of attention due to their unique properties: unlike carbon nanotubes (CNTs), all BNTs are predicted to be metallic regardless of chirality or radii. Based on density functional theory, we present a class of boron sheets, composed of mixtures of triangular and hexagonal motifs, that are more stable than any sheet-structures considered to date and thus are more likely to be the precursors of atomically thin BNTs [1]. We describe a picture of the nature of the bonding in these sheets which clarifies their stability. We further point out that our bonding picture, which focuses on the balance of two-center and three-center bonding, is crucial for the stability of other boron nanostructures. We also discuss BNTs made from our new boron sheets.

11:27AM Q31.00002 Boron Nanotubes: Characterization Through Theory  
ABHISHEK SINGH, ARTA SADRZADEH, Department of Mechanical Engineering and Materials Science, Rice University, Houston, TX 77005; BORIS YAKOBSON, Department of Mechanical Engineering and Materials Science Rice University, and Department of Chemistry, Rice University, Houston Tx 77005 — Boron nanotubes have been believed to be metallic irrespective of diameter and chirality, as opposed to carbon nanotubes (CNTs), which could be both metallic and semiconducting. However, the separation of metallic and semiconducting CNTs is still a challenging task, which eventually, plagues their applications. Using first principle calculations, we investigate mechanical and electronic properties of the BNTs and show that BNTs could also be semiconducting. We discuss the origin of semiconductivity in BNTs. Prospect of having only metallic BNTs is a great advantage over CNTs, however, having semiconducting BNTs could make them applicable in electronics, sensing and optoelectronics.

SOMILKUMAR RATHI, ASOK RAY, The University of Texas at Arlington — Ab initio calculations within the framework of hybrid density functional theory and finite cluster approximation have been performed for the electronic and geometric structures of three different types of armchair germanium carbide nanotubes from (3, 3) to (11, 11). Full geometry and spin optimizations with unrestricted symmetry have been performed. A detailed comparison of the structures and stabilities of the three types of nanotubes will be presented. The dependence of the electronic band gaps on the respective tube diameters, energy density of states, dipole moments as well as Mulliken charge distributions have been investigated. Radial buckling of tube along with bond length variations is also studied. All armchair GeC nanotubes investigated so far are semiconducting in nature. Applications in the field of nano-optoelectronic devices, molecular electronics and band gap engineering are envisioned for GeC nanotubes.

1:11PM Q31.00004 Water in nanoscale confinement: Insights into structure, dynamics, and H-NMR chemical shifts from first-principles theory  
PATRICK HUANG, ERIC SCHWEGLER, Physical Sciences Division, Lawrence Livermore National Laboratory, GIULIA GALLI, Department of Chemistry, University of California, Davis — The properties of water confined to nanoscale dimensions can differ markedly from bulk. Numerous studies of confined water focus on water in carbon nanotubes (CNTs), because CNTs provide a uniform environment with a well-defined geometry and chemical composition. However, the behavior of water in CNTs remains controversial. Here, we apply first-principles density functional theory (DFT) to study the structure and dynamics of water in CNTs, and relate our microscopic picture to experimentally-accessible observables. One such observable is H-NMR, a sensitive probe of atomic-scale structure and dynamics. While empirical procedures to relate chemical shifts to structure are known for organic molecules, analysis of NMR spectra of solids and liquids requires more sophisticated approaches. We evaluate chemical shifts of water in CNTs within periodic DFT, and relate our findings to experimental H-NMR measurements.

12:03PM Q31.00005 First-Principles Studies of Metal-Graphene and Metal-Nanotube Heterostructures  
ALEJANDRO LUGO-SOLIS, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003 — Metal-nanotube heterostructures have attracted considerable interest due to their potential applications in catalysis, fuel cell technology, and hydrogen storage. We investigate the optical properties of alkali metal atoms and clusters adsorbed on graphene and single-walled carbon nanotubes. The geometries, binding energies, and optical absorption spectra of the modeled structures are calculated in the framework of ab initio density-functional and time-dependent density-functional methods combined with the local-density approximation for the exchange-correlation functional. Our calculations show significant differences between the structures and absorption spectra of isolated alkali metal clusters and those adsorbed on graphene and carbon nanotubes.

12:15PM Q31.00006 Linear plasmon dispersion in graphene and single-wall carbon nanotubes and the influence of interlayer interactions  
R. HAMBACH, C. GIORGETTI, F. SOTTILE, L. REINING, LSI, CEA-CNRS UMR 7642-Ecole Polytechnique, France and ETSF France, C. KRAMBERGER, M.H. RÜMMELI, M. KNUPFER, J. FINK, B. BÜCHNER, T. PICHLER, IFW Dresden, Germany, E. EINARSSON, S. MARUYAMA, The Univ. of Tokyo, Dept. of Mech. Eng., 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan, K. HANNEWALD, IFTO, Friedrich-Schiller Universitaet Jena, Germany, V. OLEVANO, Institut Neel, Grenoble, France and ETSF France, A.G. MARINOPOULOS, Department of Physics and Astronomy, Vanderbilt University, Nashville, USA — Using first principle calculations [1], we studied momentum resolved electron energy loss spectra (EELS) for isolated graphene in RPA. Correspondingly, we simulated the influence of interlayer interactions on the plasmon dispersion and the importance of local field effects (or depolarization effects). The latter cause a mixing of electronic transitions resulting in a nearly linear dispersion of the plasmon in graphene for in-plane momentum transfer. Corresponding EELS measurements on isolated, vertically aligned single-wall carbon nanotubes (SWCNT) show a very similar dispersion relation along the tube axis. This validates the use of graphene to understand electronic excitations of carbon nanotubes and vice versa.

12:27PM Q31.00007 Tuning Field-Induced Energy Gap of Bilayer Graphene via Interlayer Spacing  
YUFENG GUO, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, WANLIN QIU, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154 — Using first-principles calculations, we demonstrate a sensitive dependence of the electric-field-induced energy gap of bilayer graphene on its interlayer spacing. The calculated results reveal surprisingly large (±50%) changes in the energy gap by relatively small (±10%) adjustments in the interlayer spacing near the equilibrium structure when the electric field is sufficiently high (above 3 V/nm). We elucidate the underlying mechanism by examining the response of the interlayer charge distribution to the interlayer spacing variation at different electric fields. These results suggest an effective way for reversible tuning of the field-induced energy gap of bilayer-graphene-based nanoelectronic devices through nanomechanical control.

1This work was supported by DOE Cooperative Agreement DE-FC52-06NA26274 (YFG and CFC)
12:39PM Q31.00008 Role of Surface Defects in the Carboxylation of Carbon Nanotubes: An Ab Initio Study1. NABIL AL AQTASH, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico — We investigate the mechanism of covalent sidewall functionalization of carbon nanotubes with carboxyl groups using first principles computational methods. The binding energies and equilibrium geometries of carboxylated nanotubes with no surface defects, Stone-Wales defects and vacancies are calculated in the framework of density functional theory combined with the generalized gradient approximation. Our calculations show that the binding of carboxyl groups with carbon nanotubes containing surface defects is stronger than that with defect-free nanotubes. Furthermore, the presence of carboxyl groups on the surface leads to a considerable change of the electronic and structural properties of defective nanotubes. Our results suggest that surface defects play an important role in the formation of chemical bonds between chemical groups and carbon nanotubes.

1Supported by NSF DMR-0505270.

12:51PM Q31.00009 An ab initio description of cleaning of SWNT with UV light. ABRAM VAN DER GEEST, Colorado School of Mines, KATHRINE HURST, NIST Boulder, MARK T. LUSK, Colorado Scool of Mines — The photodesorption of molecules and its application to the cleaning of single walled carbon nanotubes (SWNTs) has been experimentally demonstrated using a 248 nm laser. The excitation of the carbon nanotube π-plasmon is thought to couple to vibrational modes of the molecule-nanotube bond. An ab initio inquiry seeks to validate this hypothesis and optimize the process of nanotube cleaning. The response of SWNTs to an electric field, a description of the enhancement of surface plasmons, and the role of hot electrons are discussed.

1:03PM Q31.00010 Modeling and simulation of adhesion between carbon nanotubes and surfaces. ALPER BULDUM, NABA RAJ PAUDEL, Department of Physics, The University of Akron, Akron, OH 44325, TOSHIYUKI OHASHI, Honda Research Institute USA, Inc. Research Institute, OH 44325, COLIN BURTON, ULrice, Inc. COBE, Inc. COBE, Inc. — There have been also many experimental studies which were performed to compare the adhesion properties of carbon nanotubes with that of a gecko’s foot on smooth surfaces. Yurdumakan et al. measured the adhesive force of multiwalled carbon nanotube hairs and found it to be 200 times higher than that observed for gecko foot hairs. Here, we present theoretical investigations of CNTs interacting with surfaces. We study the deformation of CNTs and evaluate their adhesion similar to the experimental investigation of a gecko’s foot. To study the deformation behavior and adhesion of CNTs, atomistic simulations of capped armchair (10,10) nanotubes with two different lengths are performed on rigid and relaxed graphite surfaces. Simulations were also performed for different orientations of the nanotube with respect to the graphite surface to study the angular dependence of adhesion and deformation.

1:15PM Q31.00011 Monte Carlo simulations of the effect of nanotube length distribution on the percolation resistivity in single-walled carbon nanotube films. JEREMY HICKS, ASHKAN BEHNAM, ANT URAL, University of Florida — Employing Monte Carlo simulations, we generate and calculate the resistivity of multilayer films made up of single-walled carbon nanotubes with various nanotube length distributions. Each layer in the film acts as a charge-percolating 2D mesh with contacts to adjacent layers. First, we study the case when the tube-face contact resistance dominates the resistivity. For randomly oriented nanotubes, we find that, the resistivity of the film, as well as its overall percolation probability correlate strongly with the root mean square (RMS) length of the nanotubes near the percolation threshold regardless of distribution. As the nanotubes in the film become increasingly aligned, the resistivity correlation shifts to higher order in length. On the other hand, if the nanotube resistance dominates the resistivity, the resistivity of the film correlates strongly with the average nanotube length. These results, which can be explained by physical and geometrical arguments, show how individual nanotube parameters contribute to the macroscopic characteristics of the film. They also show that computational studies are an essential tool for providing insight into the percolation transport in single-walled carbon nanotube films.

1:27PM Q31.00012 Mechanism for Superelongation of Carbon Nanotubes at High Temperature1. CHUN TANG, Department of Physics & High Pressure Center, University of Nevada, Las Vegas, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics & Astronautics, CHANGFENG CHEN, Department of Physics & High Pressure Center, University of Nevada, Las Vegas — Recent discovery of super elongation of carbon nanotubes (CNTs) at high temperature raises fundamental questions about the deformation mechanism of these normally brittle materials. Here we report extensive molecular dynamics simulations that identify two key factors for this intriguing phenomenon: (1) activation of defects all over the tube at the elastic limit and continued emergence of additional defects at increasing strain that impede the formation of localized predominant instability and facilitate homogeneous deformation; (2) large-scale defect evolution that produces multistage necking and kink motion. Intricate interplay between CNT sizes and temperature activated defect nucleation and motion plays a key role in determining the overall deformation pattern.

1DOE Cooperative Agreement DE-FC52-06NA26274.

1:39PM Q31.00013 Mesoscopic model for CNT-based materials1. ALEXEY VOLKOV, KIRIL SIMOV, LEONID ZHIGILEI, University of Virginia — A mesoscopic computational model is developed for simulation of the collective mechanical and thermal behavior of carbon nanotubes (CNTs) in CNT-based materials. The model is based on a coarse-grained representation of CNTs as “breathing flexible cylinders” consisting of a variable number of segments. A novel effective “tubular” potential is developed for the description of van der Waals inter-tube interactions. Frictional forces and energy dissipation, as well as heat conduction along and between CNTs, are incorporated into the mesoscopic model and parameterized with the help of results from atomistic simulations. The developed model is used in calculations of the mechanical and thermal properties of CNT meshes and mats. The systems under consideration contain thousands of CNTs, allowing for investigation of the effective properties of CNT-based materials. The computational results are related to available experimental data.

1Support of this work is provided by NSF (NIRT-0403876) and NASA (NNX07AC41A)

1:51PM Q31.00014 First-principles studies of the switching performance of [2]rotaxane molecules and monolayers. KINYIP PHOA, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, J.B. NEATON, The Molecular Foundry, Materials Sciences Division, Lawrence Berkeley National Laboratory, VIVEK SUBRAMANIAN, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley — Density functional theory calculations of [2]rotaxane, an organic molecule consisting of a linear (straight) backbone and an encircling ring, which was recently proposed as the basis of a molecular memory device, are presented. The energy landscape describing the shifting of the ring along the backbone is calculated and carefully investigated. Furthermore, to estimate the potential RC delays associated with this molecular memory circuit, the long-wave dielectric response of [2]rotaxane monolayers is explored by applying an external field. Our calculations shed new light on the underlying working principle of this system and build on previous studies.

2:03PM Q31.00015 Structure-property relations in electronic switches based on the rotaxane and catenane supramolecular framework , YONG-HOON KIM, University of Seoul — Mechanically interlocked bistable supramolecular complexes are promising candidates of molecular electronics. Applying a multiscale computational approach combining force-fields molecular mechanics, density-functional theory, and matrix Green’s function calculations, we study the structure-property correlations in nanoelectronic switches based on [2]rotaxane and [2]catenane supramolecules. Computational aspects that increase the efficiency of charge transport characteristics calculations while ensuring the numerical accuracy will also be discussed. (This work was supported by the Korea Research Foundation Grant KRF-2007-331-C00077)

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q32 GMAG DMP: Focus Session: Molecular Magnets II Morial Convention Center 225

11:15AM Q32.00001 Strongly Correlated Electrons in the [Ni(hmp)(ROH)X]₄ Single Molecule Magnet: A DFT+U Study , CHAO CAO, Quantum Theory Project and Department of Physics, University of Florida, STEPHEN HILL, Department of Physics, University of Florida, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — The single molecule magnet [Ni(hmp)(MoOH)Cl]₄ is studied using both density functional theory and the DFT+U method, and the results are compared. By incorporating a Hubbard-U like term for both of the nickel and oxygen atoms, the experimental ground state is successfully recovered, and the exchange coupling constants derived from the DFT+U calculation fit the experimental results very well. The results show that the nickel 3d electrons and oxygen 2p electrons in this molecule are strongly correlated, and thus the inclusion of on-site Coulomb energies is crucial to obtain correct results. This work is supported by DOE DE-FG02-02ER45995 (H.-P. Cheng and C. Cao), NSF/DMR/TR-0218957 (H.-P. Cheng and C. Cao), NSF DMR0299481 (S. Hill), and NSF DMR0506946 (S. Hill). The authors want to thank NERSC, CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported within this paper.

11:27AM Q32.00002 Spin excitations in the molecule Mn₁₉ with a record ground-state spin S = 83/2 , B. BURGER, Institut für Anorganische Chemie, Universität Karlsruhe, 76128 Karlsruhe, Germany, O. WALDMANN, Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany, A.M. AKO, A.K. POWELL, Institut für Anorganische Chemie, Universität Karlsruhe, 76128 Karlsruhe, Germany, H. MUTKTA, Institut Laue-Langevin - 6 Rue Jules Horowitz, BP 156-38042, Grenoble Cedex 9, France, T. UNRUH, FRM-II, Technical University Munich, ZWE, 85747 Garching, Germany — In the magnetic molecule Mn₁₉, 12 Mn(III) and 7 Mn(II) ions are ferromagnetically coupled such as to yield a S = 83/2 ground state. We recorded Q-band ePR and inelastic neutron scattering (INS) spectra on powder samples of Mn₁₉. The ePR data is well interpreted by the model of an isolated S = 83/2 spin with uniaxial magnetic anisotropy, H = DS² + gpSB. We find D = 0.004 cm⁻¹, hence Mn₁₉ is not a single-molecule magnet. The INS spectra show a broad feature I at ca. 0.25 meV, which exhibits an uncommon temperature dependence, and two peaks II and III at ca. 3.0 and 5.7 meV. The analysis of the INS data is complicated by the huge Hilbert space of Mn₁₉, hence the behavior cannot be described in a single-spin picture, but requires an inherent many-body description.

11:39AM Q32.00003 Looking for higher anisotropy barriers in single-molecule magnets , SAIIT DATTA, University of Florida, CONSTANTINOS MILIOS, EUAÑ BRECHIN, The University of Edinburgh, U.K, STEPHEN HILL, UNIVERSITY OF FLORIDA COLLABORATION — We report single-crystal high-frequency electron paramagnetic resonance (HF EPR) studies of a series of recently discovered Mn₆ single-molecule magnets (SMMs) with large barriers to magnetization reversal. All of the complexes consist of Mn₆ triangles with a ferromagnetic interaction between them. Recent studies have shown that the exchange interactions within the triangular Mn₆ units can be switched from antiferromagnetic to ferromagnetic, resulting in a switching of the spin from S = 4 to 12 for many of the Mn₆ complexes. This strategy to “increase S” has resulted in the highest magnetic energy barrier and blocking temperature for any known SMM to date. Extensive frequency, temperature and field-orientation dependent HF EPR measurements were performed to determine the magnetic anisotropy parameters for each complex. These studies have contributed to important new insights concerning strategies for designing SMMs with high blocking temperatures, particularly for complexes containing manganese in its +3 oxidation state. 1 T. Stamatakos et al., J. Am. Chem. Soc. 129, 12505-12511, 2007.

11:51AM Q32.00004 Theory of tunneling spectroscopy in a Mn₁₂ single-electron transistor by DFT methods , LUKASZ MICHALAK, Lund University and Kalmar University, Sweden, CARLO M. CANALI, Lund University, Sweden, MARK R. PEDERSON, Naval Research Lab, Washington DC, USA, VINCENZO G. BENZA, Universita dell Insubria, Como, Italy — We present a theory of single-electron tunneling transport through a Mn₁₂ molecular magnet in the Coulomb blockade regime. We employ spin density functional theory to calculate the low-energy spin multiplet states for neutral and charged (anion and cation) Mn₁₂, split by spin-orbit interaction. Tunneling matrix elements between these states are the basic ingredients of a master equation formalism that gives the tunneling conductance as a function of the bias and gate voltage. We compare the results of this formalism with the ones obtained using a phenomenological giant-spin Hamiltonian and highlight the importance of the orbital degree of freedom included in our SDFT approach.

12:03PM Q32.00005 First-principles study of a monolayer of single-molecule magnets Mn₁₂ on a gold surface , SALVADOR BARRAZA-LOPEZ, MICHAEL C. AVERY, KYUNGWA PARK, Department of Physics, Virginia Polytechnic Institute and State University, Blacksburg VA, 24061 — Over the past decade, single-molecule magnets have drawn considerable attention due to observed magnetic quantum tunneling and interference and a possibility of using them very efficiently in devices. There have been significant experimental efforts to build and characterize thin films or monolayers of single-molecule magnets on surfaces or single-molecule magnets bridged between electrodes. In parallel, theoretical models have been proposed to understand the properties of single-molecule magnets coupled to a metal substrate. However, there do not exist atomic-scale simulations on this complex system. We simulate, within density-functional theory, prototype Mn₁₂ molecules adsorbed via a thiol group onto a gold surface. We investigate how strongly a Mn₁₂ molecule is coupled to the metal surface and how much charge and spin moments are transferred between a Mn₁₂ molecule monolayer and the metal surface. In particular, we compare the electronic and magnetic properties of the Mn₁₂ monolayer on a gold surface with those of an isolated Mn₁₂ in the presence of spin-orbit interaction. Our results may shed light into tailoring of the magnetic properties of nanomagnets as a result of electronic transfer from a proximal metallic surface.
12:15PM Q32.00006 Ignition of magnetic deflagration in Mn$_{12}$ acetate, SEAN MCHUGH, R. JAAFAR, M.P. SARACHIK, City College of New York, Y. MYASOEDOV, A. FINKLER, H. SHTIRIKMAN, E. ZELDOV, The Weizmann Institute of Science, R. BAGAI, G. CHRISTOU, University of Florida — We study the conditions for the ignition of two types of magnetic avalanches in the molecular magnet Mn$_{12}$-acetate corresponding to the major species and a fast-relaxing minor species. The major component, which has a lower anisotropy barrier, exists in these crystals at the level of 5 – 7%. The ignition temperatures are measured using small (30 × 30µm$^2$) Ge thermometers. In addition, the magnetization dynamics are measured using an array of Hall sensors of comparable size. Various aspects of the ignition will be discussed, including: the reduction of the ignition threshold due to quantum tunneling, the catalytic effect of the minor species, and the shift of the ignition point as a function of external magnetic field. The work at City College was supported by NSF grant DMR-00451605. E. Z. acknowledges the support of the Israel Ministry of Science, Culture and Sports. Support for G. C. was provided by NSF grant CHE-0414555.

12:27PM Q32.00007 Quantum Interference in the Longitudinal Oscillations of the Total Spin of a Dimeric Molecular Nanomagnet, CHRISTOPHER RAMSEY, ENRIQUE DEL BARCO, University of Central Florida, STEPHEN HILL, University of Florida, SONALI SHAH, CHRISTOPHER BEEDLE, DAVID HENDRICKSON, University of California at San Diego — The synthetic flexibility of molecular magnets allows one to systematically produce samples with desirable properties such as those with entangled spin states for implementation in quantum logic gates. Here we report direct evidence of quantum oscillations of the total spin length of a dimeric molecular nanomagnet through the observation of quantum interference associated with tunneling trajectories between states having different spin quantum numbers. As we outline, this is a consequence of the unique characteristics of a molecular Mn$_{12}$ wheel which behaves as a (weak) ferromagnetic exchange-coupled molecular dimer: each half of the molecule acts as a single-molecule magnet (SMM), while the weak coupling between the two halves gives rise to an additional internal spin degree of freedom within the molecule, namely that its total spin may fluctuate. This extra degree of freedom accounts for many magnetization tunneling resonances that cannot be explained within the usual giant spin approximation. More importantly, the observation of quantum interference provides unambiguous evidence for the quantum mechanical superposition involving entangled states of both halves of the wheel.

12:39PM Q32.00008 EPR Studies of Magnetically Dilute Ga-Doped Single Crystals of Fe$_{15}$ Antiferromagnetic Molecular Wheels, JOHN HENDERSON, CHRISTOPHER RAMSEY, ENRIQUE DEL BARCO, University of Central Florida, THEODOROS STAMATATOS, GEORGE CHRISTOU, University of Florida — Studies of the quantum dynamics of the electron spins in solid state systems has gained considerable interest recently due to their potential for use as quantum computing substrates. One class of materials, molecular magnets, are of particular importance, owing to the seemingly limitless array of spin configurations due to synthetic chemical flexibility. Efforts are currently devoted to minimizing decoherence times by diminishing dipolar effects. In this regard, we have carried out EPR measurements on small single crystals of 0.5% Ga doped Fe$_{18}$ molecular antiferromagnetic wheels at temperatures down to 300 mK using planar resonators patterned on GaAs wafers. This system constitutes a dilute sample of $S = 3/2$ molecules dispersed within a sea of $S = 0$ (at low temperature) molecules, which significantly reduces dipolar interactions and might provide a means of observing Rabi oscillations in crystals of molecular magnets. Detailed angular dependence studies reveal significant anisotropy with D = 500 mK and E = 20 mK. The presence of second order anisotropy (E) is very unusual for such a high symmetry system and its interpretation will be discussed. Pulsed-EPR measurements and doping concentration dependence will also be discussed.

12:51PM Q32.00009 Spin-Jahn-Teller effect in the antiferromagnetic molecular wheel CsFe$_8$, O. WALDMANN, Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany, L. SCHNELZER, B. PILAWA, Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany, M. HORVATIC, Grenoble High Magnetic Field Laboratory, CNRS, BP 166, 38042 Grenoble Cedex 9, France — In an antiferromagnetic (AF) molecular wheel, magnetic metal ions are clustered together by organic ligands such as to form rings. Due to AF Heisenberg interactions in the wheel, the molecule’s ground state at zero magnetic field is nonmagnetic with total spin $S = 0$. The higher lying states belong to $S = 1, 2, ...$. In this magnetic field these states are Zeeman split, leading to a series of level-crossings (LCs) at characteristic fields at which the ground state changes from $S = 0$, $M = 0$ to $S = 1$, $M = 1$, and so on. Hence, via the field, the magnetic ground state of the molecule can be tuned through a degeneracy at the LC. Field-dependent measurements of the magnetic torque and $^1$H-NMR on CsFe$_8$ single crystals were performed, which show clear indications of a phase transition at the LCs at low temperatures [PRL 96, 027206 (2006); PRL 99, 087201 (2007)]. These phase transitions are explained by a field-induced spin-Jahn-Teller effect (JTE) due to tunneling of the field and the lattice: For fields close to a LC, a spontaneous structural distortion of the CsFe$_8$ wheel occurs such as to lift the degeneracy in the magnetic energy spectrum, hence the spin-JTE.

1:03PM Q32.00010 Magneto-infrared investigations of $[\text{MoO}_4\text{O}_{30}(\mu_2-\text{OH})_{18}]^{8-}$, $\text{H}_2\{\text{Ni}^{II}_4(\text{H}_2\text{O})_4\}_4\}$, J. CAO, J.L. MUFSELD, University of Tennessee, M. PEDERSON, Naval Research Laboratory, R. KLEMM, University of Central Florida, P. KOGERLER, Ames Laboratory — We measured the magneto-infrared spectrum of $[\text{MoO}_4\text{O}_{30}(\mu_2-\text{OH})_{18}]^{8-}$, $\text{H}_2\{\text{Ni}^{II}_4(\text{H}_2\text{O})_4\}_4$ in order to test the suggestion that molecular structure (and thus interactions between spins) may be changing with applied magnetic field. Although this low-noise magneto-infrared work was done in a superconducting magnet (which limits the field range to only 18 T), these experiments do provide direct evidence for small field-induced local distortions of the lattice. The field-induced change in the localized $\text{H}_2\text{O}$ wagging mode on the O attached to the Ni sites is particularly evident. This result is consistent with previous magneto-optics work indicating a small change in the Ni$^{II}_4$ crystal field environment at 30 T. We also consider whether the magneto-infrared results and the consequent small implied changes in local structure with magnetic field are enough to account for the observed magnetization data, and we discuss complementary mechanisms based on more extended spin Hamiltonians that may also account for large changes in J and D in molecular-based magnets.

1:15PM Q32.00011 Dzyaloshinskii-Moriya interactions and multiferroic behavior in high-symmetry single molecule magnets, RICHARD KLEMM, University of Central Florida, DMITRI EFREMOV, Technische Universität Dresden — We study analytically the effects of the antisymmetric exchange, or Dzyaloshinskii-Moriya interactions in high-symmetry single molecule magnets with 2-4 magnetic ions per cluster. When the Moriya rules allow it, such as when an ionic bond does not contain a center of inversion, these interactions can lead to interesting observable effects, including the presence of an electric polarization driven by an applied magnetic field, and associated multiferroic behaviors. We will present our results for tetramers with the common $S_1$ molecular group symmetry, and for other ultrasmall single molecule magnets.

1:30PM Q32.00012 Spin echo experiments on dilute ensembles of single molecule magnets, GREGOIRE DE LOUBENS, ANDREW D. KENT, NYU, Physics, VLADIMIR KRYMOV, GARY J. GERFEN, Yeshiva University, AECOM, Physiology & Biophysics, CHRIS C. BEEDLE, DAVID N. HENDRICKSON, UCSD, Chemistry & Biochemistry — Single molecule magnets (SMMs) have been suggested as candidates for qubits in quantum processors. However, the coherence time ($T_2$) of high-spin molecules has not been determined. In SMM single crystals the strong dipolar interactions between molecules (separated by only 1 nm) is expected to drastically reduce the coherence time. In order to determine the coherence time, $T_2$, we undertook a series of experiments. In particular, dilute frozen solutions of the SMM Ni$_4$ have been studied using high frequency D-band (130 GHz) EPR setup [1]. Despite the random orientation of the molecules, well defined EPR absorption peaks are observed, due to the strong variation of the splittings between the different spin-states on magnetic field. Temperature dependent studies (> 4 K) and comparison with simulations enable identification of the spin transitions and determination of the Hamiltonian parameters, found to be close to those of Ni$_4$ single crystals. The absence of echo in pulsed experiments sets an upper bound of about 50 ns on the spin coherence time in Ni$_4$ at 130 GHz and T = 5.5 K. [1] G. de Loubens et al., arXiv:0709.2146.
1.39PM Q32.00013 Transition Metal Dimers and Physical Limits on Magnetic Anisotropy, TOR OLOF STRANDBERG, CARLO M. CANALI, Kalmar University, ALLAN H. MACDONALD, University of Texas at Austin — Recent advances in nanoscience have raised interest in the minimum bit size required for classical information storage, i.e. for bistability with suppressed quantum tunnelling and energy barriers that exceed ambient temperatures. In the case of magnetic information storage much attention has centred on molecular magnets with bits consisting of 100 atoms, magnetic uniaxial anisotropy energy barriers 50 K, and very slow relaxation at low temperatures. In our recent article (Nature Materials 6, 648 - 651 (2007)), we draw attention to the remarkable magnetic properties of some transition metal dimers which have energy barriers approaching 500 K with only two atoms. The spin dynamics of these ultra small nanomagnets is strongly affected by a Berry phase which arises from quasi-degeneracies at the electronic Highest Occupied Molecular Orbital (HOMO) energy. In a giant spin-approximation, this Berry phase makes the effective reversal barrier thicker.

1.51PM Q32.00014 Magnetic anisotropies of late transition metal atomic clusters, JAIME FERRER, LUCAS FERNANDEZ-SEIVANE, Departamento de Física, Universidad de Oviedo — We analyze the impact of the magnetic anisotropy on the geometric structure and magnetic ordering of small atomic clusters of palladium, iridium, platinum and gold. We have employed a non-collinear implementation of Density Functional Theory where the spin-orbit interaction has been included self-consistently. The size of the clusters range from two to five, six or seven atoms, depending on the element. Our results highlight the relevance of the spin orbit interaction in the magnetic properties of small atomic clusters made of fourth- and fifth-row elements [1].

2:03PM Q32.00015 Dirac Equation for Electrodynamical Model Particle, J.X. ZHENG-JOHANSSON, IOFPR — We set up the Maxwell’s equations and subsequently the classical wave equations for the electromagnetic waves which together with their generating source, an oscillatory charge of zero rest mass, make up a particle travelling at velocity $v$ as with the charge in the fields of an external scalar and vector potentials. The direct solutions in constant external field are Doppler-displaced plane waves propagating at the velocity of light $c$; at the de Broglie wavelength scale and expressed in terms of the dynamically equivalent and appropriate geometric mean wave variables, these render as functions identical to the space-time functions of the Dirac spinor, and these are identical to the de Broglie phase waves given previously from explicit superposition. For two spin-half particles of a common set of space-time functions constrained with antisymmetric spin functions as follows the Pauli principle for same charges and as separately indirectly induced based on experiment for opposite charges, the complete wave functions are identical to a Dirac spinor. The back-substitution of the so explicitly determined complete wave functions in the corresponding classical wave equations of the two particles, subjected further to reductions appropriate for the stationary-state particle motion and to rotation invariance when in three dimensions, give a Dirac equation set; the procedure and conclusion are directly extendible to arbitrarily varying potentials by use of the Furious theorem and to three dimensions (full paper: QT55).

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q33 GMAG FIAP DMP: Focus Session: Spin Polarization in Compound Semiconductors
Morial Convention Center 224

11:15AM Q33.00001 Boundaries Between Current Carrying Semiconductors and Metallic Contacts, INANC ADAGIDELI, Universitaat Regensburg — No abstract available.

11:51AM Q33.00002 Current-Induced Spin Polarization in Gallium Nitride, W. KOEHL, C. POBLENZ, M.H. WONG, U. MISHRA, J. SPECK, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Recent experimental studies have shown that when a current is passed through certain non-centrosymmetric semiconductors (GaAs, ZnSe), a net spin polarization may be generated throughout the material. However, the physical mechanism responsible for this phenomenon, known as current-induced spin polarization (CISP), is still poorly understood but known to exist at high temperatures in wide-bandgap semiconductors [1]. In order to further explore the degree to which CISP depends on the band structure and spin lifetimes of a material, we measure the phenomenon in GaN, a wide-bandgap, non-centrosymmetric semiconductor. A series of n-type GaN epilayers are grown in the wurzite phase via molecular beam epitaxy at a variety of doping densities chosen to modulate the transverse spin lifetime, $T_\perp$, across its full available range. Using the Kerr effect, CISP is then characterized in these epilayers as a function of excitation energy over a range of temperatures.


1Work supported by the NSF and ONR.

12:03PM Q33.00003 Spin polarization in quantum point contact structures, ANH NGO, SERGIO ULLOA, Department of Physics and Astronomy, Ohio University — One of the important goals in the field of spintronics is to produce spin-polarized currents in semiconductors [1]. The Rashba spin-orbit interaction is useful in this regard, because its strength is controllable by applying an electric field. In this work we study ballistic transport through semiconductor quantum point contact systems under different confinement geometries and applied fields. In particular, we investigate how the lateral spin-orbit coupling, as induced by the lateral confinement potential, plays a non-trivial role on the spin polarization of the current, even in the absence of magnetic field. We find that high spin polarization can be obtained by controlling the asymmetric shape of the confinement potential, and contrast our results with previous work in the literature [2]. This behavior suggests a novel scheme to implement spin-filters without external magnetic fields, and we present its dependence on structural parameters.


12:15PM Q33.00004 All-Electric Quantum Point Contact Spin Polarizer, PHILIPPE DEBRAY, SAY-DUR RAHMAN, University of Cincinnati, Cincinnati, OH 45221, STEVEN HERBERT, Xavier University, Cincinnati, OH 45207, MARC CAHAY, RICHARD NEWROCK, University of Cincinnati, Cincinnati, OH 45221 — The conductance of InAs quantum point contacts (QPCs), created by two side gates on InAs/InGaAs quantum-well structures, was measured at low temperatures (≤ 4.2K) as a function of Fermi energy. By tuning the bias voltages of the gates, we were able to make appear or disappear on demand a conductance plateau at $G \cong 0.5 (2e^2/h)$. The presence of this plateau indicates complete spin polarization in the fundamental mode of transport. The 0.5 plateau appears when the transverse confining potentials of the QPC are tuned to be highly asymmetric. We believe the spin polarization responsible for the 0.5 plateau is induced by the lateral spin-orbit coupling, which originates from the transverse electric field of the confining potentials at the edges of the QPC. In a strong perpendicular magnetic field the magnetic confinement screens out the electrostatic confinement and the 0.5 plateau disappears. Our results show that it is possible to use an InAs QPC as a spin polarizer of both spin species through appropriate tuning of the bias voltages of its side gates.

2This work is supported by the National Science Foundation under grant ECCS-0725404
12:27PM Q33.00005 Nanomechanical spin-polarizer, ALEXEY KOVALEV, LIVIU ZĂRBO, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA, YAROSLAV TŠERKVONYAK, Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA, GERRIT BAUER, Kavli Institute of NanoScience, Delft University of Technology, Lorentzweg 1, 2628CD Delft, The Netherlands, JAIRO SINOVA, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We study the effects of time dependent strain on transport properties in a long semiconductor rod and predict a piezo-spin effect. Torsional oscillations of a free-standing semiconductor beam are shown to cause spin-dependent oscillating with time potentials that spin-polarize an applied charge current in the presence of intentional or disorder scattering potentials. One may apply AC voltage synchronized with the mechanical motion to obtain a DC spin current. The thus created spin accumulation in the leads can be detected by e.g. ferromagnetic side contact or by the optical Kerr rotation. We propose to build the mechanical spin generators and manipulators based on the piezo-spin effect.

12:39PM Q33.00006 Generation and Decay of Spin Flip Waves in a CdMnTe Quantum Well, P. JACOBS, R. MERLIN, U. Michigan, Ann Arbor, MI, C. AKU-LEH, F. PEREZ, INSP, UMR 7588, CNR/Paris VI et VII, France, G. KARCZEWSKI, Polish Academy of Sciences, Warsaw, Poland — Recently, two dimensional electron gases (2DEG) embedded in semimagnetic Cd$_{1-x}$Mn$_x$Te quantum wells have been introduced as a model for spin-polarized systems. The addition of a small amount of Mn induces a giant Zeeman splitting such that, under moderate magnetic fields, spin effects dominate over orbital quantization, providing the reverse situation to that of GaAs. Using Raman spectroscopy, both collective and single-particle spin excitations have been observed in CdMnTe [1]. We have used ultrafast pump-probe spectroscopy to study collective spin-flip excitations in modulation doped CdMnTe quantum wells. Oscillations due to the zone center spin-flip wave were generated by circularly-polarized 70fs pump pulses and detected by Kerr rotation of linearly-polarized probe pulses. The spin-flip lifetime has a strong dependence on the applied magnetic field and also by weak heating due to laser absorption. The dependence of the lifetime on excitation energy and magnetic field indicate that the optically-excited heavy holes and their spin orientation play an important role in the decay of the collective mode. [1] F. Perez et al., Phys. Rev. Lett. 99, 026403 (2007)

12:51PM Q33.00007 Quantum Anomalous Hall Effect in HgMnTe Quantum Wells, CHAOXING LIU, Center for Advanced Study, Tsinghua University, Beijing, 100084, China, XIAOLIANG QI, Department of Physics, McCullough Building, Stanford University Stanford, CA 94305, XI DAI, ZHONG FANG, Institute of Physics, Chinese Academy of Sciences Beijing, 100084, China, SHOUCHENG ZHANG, Department of Physics, McCullough Building, Stanford University Stanford, CA 94305 — Quantum Hall effect is usually observed in the two-dimensional electron gas with an external magnetic field, where the electronic states form Landau levels. In this work, we show that a new phenomenon, the quantum anomalous Hall effect, can be realized in HgMnTe quantum wells, without the external magnetic field and associated Landau levels. This effect originates purely from the magnetization of Mn atoms, and is closely related to the quantum spin Hall effect observed in HgTe quantum wells recently. The opposite signs of sp-d exchange coupling between the Mn atoms and conduction or valence band electrons is crucial for realizing this effect. The quantized Hall conductance is predicted for a range of Mn concentrations and the relative magnitude of Mn atoms. Between the experimentally accessible parameter regime, we propose an experiment to demonstrate that the quantized Hall conductance indeed arises from the Mn magnetic moments rather than Landau levels. This effect enables dissipationless charge current in spintronics devices.

1:03PM Q33.00008 The Effect of Detector Bias on Non-Local Measurements of Spin Transport, E.S. GARLID, T. KONDO, University of Minnesota, K.S.M. REDDY, Q. HU, P.A. CROWELL, C.J. PALMSTRØM, University of Minnesota — Previous studies of spin transport in Fe/GaAs heterostructures have observed a strong non-monotonic dependence of the spin polarization on the bias across the injector contact in a non-local measurement. We have studied the dependence of the non-local voltage signal in Fe/GaAs/Fe spin valves as a function of detector bias. Measurements were made on lateral devices fabricated from epitaxial Fe/n-/n-GaAs heterostructures that have observed a strong non-monotonic dependence of the spin polarization on the bias across the injector contact in a non-local measurement. We have studied the dependence of the non-local voltage signal in Fe/GaAs/Fe spin valves as a function of detector bias. A sign change was observed at both forward and reverse detector bias, and the detector sensitivity was enhanced by up to a factor of five under large forward bias. This enhanced sensitivity may reflect the energy dependence of the Fe/GaAs interfacial density of states, although the connection between charge and spin transport in the semiconductor channel must also be considered. This work was supported by ONR and the NSF MRSEC, IGERT, and NNNM programs.

1:15PM Q33.00009 Growth and Characterization of VLS-type (Zn,Mn)Se nanowires, BENJAMIN COOLEY, Dept. of Physics and Materials Research Institute, Penn State University, TREVOR CLARK, Materials Research Institute, Penn State University, NIRMAL P. SAMPARTH, Dept. of Physics and Materials Research Institute, Pennsylvania State University — Magnetically-doped semiconductor nanowires offer an interesting regime for exploring carrier-induced ferromagnetism in the presence of a 1D density of states. Measurements were performed by biasing the detector electrode with respect to a reference electrode and using lock-in techniques to measure the spin polarization generated from an AC biased injector electrode. The non-local voltage signal was found to have a very different dependence on detector bias than on injector bias. A sign change was observed at both forward and reverse detector bias, and the detector sensitivity was enhanced by up to a factor of five under large forward bias. This enhanced sensitivity may reflect the energy dependence of the Fe/GaAs interfacial density of states, although the connection between charge and spin transport in the semiconductor channel must also be considered. This work was supported by ONR and the NSF MRSEC, IGERT, and NNNM programs.

1:27PM Q33.00010 Enhancement of In-Plane Magnetic Anisotropy Through Compensation in Ga$_{1-x}$Mn$_x$P:S, P.R. STONE, O.D. DUBON, University of California, Berkeley and Lawrence Berkeley National Lab, K.M. YU, J.W. BEEMAN, Lawrence Berkeley National Lab, C. BIHLER, M.S. BRANDT, Walter Schottky Institut, Technische Universitat Munchen — Ga$_{1-x}$Mn$_x$P is a ferromagnetic semiconductor (FS) in which exchange is mediated by localized holes [Scarpulla et al., Phys. Rev. Lett. 95, 207204 (2005)]. As is the case for the prototypical FS Ga$_{1-x}$Mn$_x$As, there exists a uniaxial magnetic anisotropy between in-plane $<$110$>$-type directions with the magnetic easy axis lying near the in-plane [1-10] direction [Bihler et al., Phys. Rev. B 75, 214419 (2007)]. Here we report the effect of compensation of Mn acceptors by sulfur donors on the in-plane uniaxial magnetic anisotropy in Ga$_{1-x}$Mn$_x$P as measured by both ferromagnetic resonance (FMR) and SQUID magnetometry. Raising the S concentration increases the magnitude of the uniaxial magnetic anisotropy between in-plane $<$110$>$-type directions. While the [1-10] direction remains the easy axis in the plane of the film, “wasp-waisted” hysteresis loops develop in the [110] direction as the S concentration increases. The wasp-waisted loops are modeled whereby magnetization reversal occurs by a combination of coherent spin rotation and noncoherent spin switching. Finally, by comparing FMR and SQUID data we extract domain wall formation energies as a function of compensation.
1:39PM Q33.00011 Deposition and characterization of highly spin-polarized $\text{Co}_{1-x}\text{Fe}_x\text{S}_2$ thin films.\textsuperscript{1}, MICHAEL MANN0, C. LEIGHTON, University of Minnesota — Many spintronic devices could benefit from the use of a highly spin polarized ferromagnet. We have recently demonstrated tunable spin polarization of $-56 < P < +85\%$ by composition control of the Fermi level in bulk $\text{Co}_{1-x}\text{Fe}_x\text{S}_2$.\textsuperscript{1} Although this material offers great promise for fundamental studies of spintronic devices, integration in devices such as spin injectors requires deposition of thin films. We present here synthesis details, structural, electronic, and magnetic properties of polycrystalline $\text{Co}_{1-x}\text{Fe}_x\text{S}_2$ films successfully fabricated by \textit{ex-situ} sulfidation on $\text{Al}_2\text{O}_3$ (0001), $\text{SrTiO}_3$ (001), and GaAs (001). The synthesis involves exposure of sputter or MBE deposited Co and Co-Fe alloy films to a S atmosphere at various reaction temperatures. Significant reaction with S occurs only above 200°C, while at 350°C and above we observe single-phase $\text{Co}_2\text{S}_2$ XRD patterns, and S contents (from EDS) of 65-70%. The conversion process has been studied in detail using multiple probes. Optimal conditions produce films that are ferromagnetic with the bulk $T_C$, bulk magnetization, metallic transport, and the expected magnetotransport phenomena. [1] L. Wang et al., Phys. Rev. B. 73 144402 (2006).

\textsuperscript{1}Work supported by NSF MRSEC.

1:51PM Q33.00012 Spin-filtering properties of ultra thin Eu chalcogenide films\textsuperscript{1}, MARTINA MUELLER, MARIUS COSTACHE, JAGADEESH MOODERA, Francis Bitter Magnet Lab, MIT — Promising materials for the generation of nearly fully polarized current are the magnetic semiconductors $\text{EuO}$ and $\text{EuS}$ when used as tunnel barriers. The spin-filter effect is due to exchange splitting of their conductance band below the ferromagnetic transition temperature, $T_C$. Combined with a structural and electrical compatibility with Si, Eu chalcogenides can be recognized as potential materials to study spin injection into semiconductors. In this work, special attention was drawn to the magnetic and transport properties of thin (<6nm) $\text{EuO}$ and $\text{EuS}$ films to explore the feasibility of their integration into spin-injection devices. We investigated the magnetic, structural and transport behavior of $\text{EuO (EuS)}$ thin films with regard to thickness- and substrate-induced changes. The influence of reduced dimensionality on exchange splitting and spin filter efficiency was observed in transport experiments using $\text{EuO (EuS)}$ as a tunnel barrier. “The phenomena of spin filter tunneling”, J. S. Moodera, T. S. Santos and T. Nagahama, J. Phys.: Condens. Matter 18 (2007) 1–24 – A review

\textsuperscript{1}Work supported by NSF and ONR research funds.

2:03PM Q33.00013 Resonant spin dipole induced by an in-plane potential gradient spin-orbit interaction\textsuperscript{1}, C. S. CHU, K. Y. CHEN, Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, A. G. MAL’SHUKOV\textsuperscript{2}, Institute of Spectroscopy, Russian Academy of Science, 142190 Troitsk, Moscow oblast, Russia — Spin-orbit interaction (SOI) arising from in-plane potential gradient is invoked for the generation of spin accumulation in a driven electric field. The SOI and a local in-plane potential pattern together bring about resonant spin dependent scatterings to electrons in a nonequilibrium distribution. In the vicinity of a ring-shaped potential barrier pattern, a spin dipole distribution with a resonant dipole strength characteristic is obtained. As the chemical potential $\mu$ dependent scatterings to electrons in a nonequilibrium distribution.

\textsuperscript{1}Work supported by the National Science Council of R.O.C., Taiwan

\textsuperscript{2}also affiliates with the National Chiao Tung University
12:03PM Q35.00003 Electronic Structure of Conduction Bands in Strained Si Nanomembranes
C. EUARUKSAKUL, Z. LI, C.S. RITZ, B. TANTO, D.M. COTTRILL, M.-H. HUANG, F. CHEN, D.E. SAVAGE, University of Wisconsin-Madison, F. LIU, University of Utah, F.J. HIMPSEL, M.G. LAGALLY, University of Wisconsin-Madison — We observe energy shifts of several conduction bands and a splitting of the conduction band minimum in elastically strained Si(001) and Si(110) Si nanomembranes (NMs) using X-ray absorption spectroscopy from the Si 2p core level. The surface sensitivity of absorption spectroscopy with electron yield detection makes the method suitable for studying very thin strained layers. Elastically strained NMs are dislocation free and thus provide an excellent model for determining the relationship of energy levels and strain. We measure the change in the global conduction band minima near the six X-points and also higher minima at the L and I' points, which yield information about the direction of the absolute energy shift due to the strain. Quantitative values of the level positions, including the core levels, are provided and compared to theory.

1Research supported by DOE, NSF and AFOSR.

12:15PM Q35.00004 Inelastic Electron Tunneling Spectroscopy Study of MOS Diodes Based on High-k Gate Dielectrics
S.L. YOU, C.C. HUANG, C.J. WANG, H.C. HO, J. KWO, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, W.C. LEE, K.Y. LEE, Y.D. WU, Y.J. LEE, M. HONG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan — Inelastic electron tunneling spectroscopy was applied to characterize the microstructure, interface, and trap-related states in silicon MOS diodes made of high k gate dielectrics HfO₂, Y₂O₃, and stacked HfO₂/Y₂O₃ bilayers by molecular beam epitaxy and atomic layer deposition under various heat treatments. Reproducible vibrational modes of monolonic HfO₂ and cubic Y₂O₃ were identified from IETS spectra. The gate bias dependence of the spectrum enables to ascribe the phonon modes adjacent to the lower or upper interface. A simple modeling was employed to analyze the trap related features in the spectra of stacked HfO₂/Y₂O₃ bilayers, and showed that most traps are located near the HfO₂/Y₂O₃ interface due to dissimilar charge distributions of two ionic oxides of different cation valences, and the interfacial strains of dissimilar structures. Work is now extended to Y-doped HfO₂ films in cubic phase with an enhanced k over 30.

12:27PM Q35.00005 On the role of Al doping at the SiO₂/HfO₂ interface
ONISE SHARIA, A.A. DEMKOV, UT Austin, G. BERSUKER, B.H. LEE, SEMATECH — One of the main challenges associated with the integration of high-k gate dielectrics such as hafnia is the identification of metal electrodes exhibiting the work function aligned with Si band edges. Due to the inherent instability of metals in contact with hafnia under high temperature, the focus has recently shifted towards developing a metal gate stack with appropriate effective work functions (EWF), which would result in the required low transistor threshold voltage. In this talk we report the theoretical results on doping the SiO₂/HfO₂ gate stack with Al atoms which, as we show, controls the EWF. We consider several dopant-vacancy models in various positions with respect to the interface. The proper stoichiometry avoiding fixed charge is maintained in all models. We find that doping at the interface has lower energy than doping in the bulk of silica or hafnia, which suggests the segregation of Al atoms towards the interface. Importantly, in all cases Al-vacancy complexes at the interface significantly change the band alignment, reducing the valence band offset. Thus, doping the SiO₂/HfO₂ gate stack with Al atoms offers a consistent way to adjust the alignment. This increase of the EWF can be explained with our previously introduced model that suggests that an oxygen depleted interface provides less effective screening, which in turn increases the interface dipole.

12:39PM Q35.00006 Oxide charge and band alignments in Pt/epi-Lu₃O₅/Si (111) structures studied by Internal Photoemission and C-V measurements
W. CAI, J.P. PELZ, Ohio State Univ., C. ADAMO, D.G. SCHLOM, Pennsylvania State Univ. — A variety of rare-earth/transition metal oxide films (of interest as possible “high-k” gate dielectrics for future MOS devices) were found to have similar band gap and band alignments to Si, and “tailing” conduction band (CB) states extending ~1 eV below the “primary” CB [1]. We used internal photoemission/photoconductivity (Int-PE/PC) and capacitance-voltage (C-V) measurements to study 20 nm-thick epitaxial Lu₂O₃ film grown at 700 °C on Si(111). A ~1.5V difference between the oxide- and Si- flat band voltages (measured by PC and C-V respectively) indicates ~6 × 10¹² cm⁻² fixed positive oxide charge, which was mostly removed by a ~350 °C post-metallization vacuum anneal. Int-PE measurements indicate the CB measured from the metal-side lines up ~0.4 eV below the “primary” CB measured from the Si side, in contrast with our finding on Pt/epi-SiO₂/Si (111) [2] that the metal-side CB aligned with the tail-state CB. Also, Ballistic Electron Emission Microscopy of Pt/epi-Lu₂O₃/Si (111) found ~0.3 - 0.4 eV higher energy barrier than found by Int-PE, suggesting significant transient charge trapping in this sample. Work supported by NSF Grant No. DMR-0505165. [1] V. V. Afanas’ev et al., Appl. Phys. Lett. 85, 5917 (2004); 88, 032104 (2006). [2] W. Cai et al., Appl. Phys. Lett. 91, 042901 (2007).

12:51PM Q35.00007 Electrical and optical properties of Pt/Si thin films
HENDRIK BENTMANN, A.A. DEMKOV, UT Austin, STEFAN ZOLLNER, RICH GREGORY. Freescale Semiconductor — Metal silicides are used in complementary metal-oxide-semiconductor devices (CMOS) to form contacts between metal interconnects and source, drain, and gate silicon of the transistors. They offer important properties like low resistivity, low contact resistance to Si as well as excellent process compatibility with the standard Si technology. Recently, metal silicides have attracted renewed attention and they are a current research topic in the semiconductor industry. We report a joint theoretical and experimental study of thin Pt silicide films. Employing density functional theory (DFT) methods we have investigated the electronic structure as well as bonding and optical properties of PtSi and Pt₅Si. Additionally, we have calculated surface energies for various orientations and terminations of PtSi surfaces. Our results suggest the work function aligned with Si band edges. Due to the inherent instability of metals in contact with hafnia which yield information about the direction of the absolute energy shift due to the strain. Quantitative values of the level positions, including the core levels, which were identified with inter-band transitions in the d-manifold of platinum and compared to theory.

1:03PM Q35.00008 Ab-initio study of early stages of III-V epitaxy on Si: direct vs. buffer deposition on vicinal surfaces
A.A. DEMKOV, ONISE SHARIA, HENDRIK BENTMANN, UT Austin — III-V materials, such as GaAs or InSb as well as other compound semiconductors with high carrier mobility are considered as potential candidates for a channel material in future CMOS-type devices. The most promising route to incorporate these advanced materials into CMOS is by growing epitaxial thin films on Si, either directly or via a buffer layer. Direct deposition suffers from a large lattice mismatch, and domain formation caused by the presence of steps on the Si surface. Perovskite oxides such as SrTiO₃ (STO) offers a possibility to reduce the lattice mismatch between Si and, e.g. GaAs in a step-wise fashion, however, the steps on the semiconductor surface present a somewhat unusual challenge. On the other hand, the use of vicinal surfaces for the direct deposition of GaAs on Si may eliminate the problem of orthogonal domains. Thus understanding the role of steps during the crystal growth is key to both approaches. In this talk we report a theoretical study of STO epitaxy on the vicinal Si(001) surface. In particular, we find that at the early stages of growth, Sr adatoms segregate to the step edges. We also consider the direct epitaxy of III-V compound semiconductors on high index Si surfaces, specifically, the silicon (112) surface. We consider In adsorption on this surface and identify a stable 7x1 substitutional reconstruction which is fundamentally different from the 6x1 reported for Ga. 
1:15PM Q35.00009 Atomic-layer-deposited HfO$_2$ on In$_{0.53}$Ga$_{0.47}$As – passivation and energy-band parameters...Y.C. CHANG, K.Y. LEE, M.L. HUANG, Y.J. LEE, T.D. LIN, M. HONG, Dept. of Materials Science and Engineering, National Tsing Hua University, Taiwan, J. KWO, Dept. of Physics, National Tsing Hua University, Taiwan — High k dielectric HfO$_2$ films were deposited by atomic-layer deposition on air-exposed In$_{0.53}$Ga$_{0.47}$As/InP (100), and found to exhibit an atomicly sharp interface free of arsenic oxides, an excellent aspect for Fermi level pinning. Angular-resolved x-ray photoelectron spectroscopy (XPS) using synchrotron radiation, however, observed the existence of Ga$_2$O$_3$, In$_2$O$_3$, and In(OH)$_3$ at the interface. The I-V of the MOS diode for an HfO$_2$ 7.8 nm thick follows the Fowler-Nordheim tunneling mechanism with a low leakage $\sim 10^{-8}$A/cm$^2$ at V$_{FB}$+1V, and an interfacial density of states $D_{it}$ of $2x10^{12}$cm$^{-2}$eV$^{-1}$. A conduction-band offset of $\sim$ 1.8 eV, and a valence-band offset of $\sim$ 2.9 eV were derived from the transport, and XPS data, respectively. For another HfO$_2$ film 4.5nm thick we achieved a CET value as small as 1.0nm, and a leakage of 3.8x10$^{-10}$A/cm$^2$ at V$_{FB}$+1V. The good scalability of ALD grown HfO$_2$ film with low leakage makes it very promising for III-V MOSFET applications.

1:27PM Q35.00010 Interfacial-layers-free Ga$_2$O$_3$(Gd$_2$O$_3$)/Ge MOS Diodes, C.H. LEE, T.D. LIN, K.Y. LEE, M.L. HUANG, L.T. TUNG, M. HONG, Department of Materials Science and Engineering, National Tsing Hua University, Taiwan, J. KWO, Department of Physics, National Tsing Hua University, Taiwan — High k dielectric Ga$_2$O$_3$(Gd$_2$O$_3$) films were deposited directly on Ge by Molecular-Beam-Epitaxy without the employment of GeON interfacial layer. Excellent electrical properties, such as a high k value of 14.5, a low leakage current density of only 3x10$^{-9}$A/cm$^2$ at V$_{FB}$+1 V, and a high mobility of 800 cm$^2$/V·s were obtained after 530°C oxidation in N$_2$ ambient for 5 min. An abrupt Ga$_2$O$_3$(Gd$_2$O$_3$)/Ge interface was revealed by high-resolution transmission electron microscopy as well as in-situ x-ray photoelectron spectroscopy (XPS). Detailed XPS studies indicate that the oxide/Ge interface consists of mainly Ge-O-Gd bonding, distinctly different from that of native oxide. Furthermore, the 500°C annealing did not change the chemical bonding, implying a great thermodynamic stability of the hetero-structure. The outstanding electrical and thermodynamic properties qualified Ga$_2$O$_3$(Gd$_2$O$_3$) as a promising dielectric for Ge and proved the GeON interfacial layer to be unnecessary.

1:39PM Q35.00011 Aspect Ratio Study of Microstructures Formed using an Adaptable Photomask, ANNA FOX, ADAM FONTECCHIO, Drexel University — We present an aspect ratio study of microstructures fabricated using a holographically formed polymer dispersed liquid crystal (H-PDLC) adaptable photomask. Recently it has been shown that H-PDLC films can act as electrically controllable light valves to selectively allow transmission of UV exposure in the lithographic process, making it ideal for application as a reconfigurable photomask. This study focuses on comparing aspect ratios of structures patterned using this adaptable photomask and processed with wet etching and reactive ion etching techniques. Aspect ratio comparisons with structures fabricated using a binary mask and etched using an identical process are presented. Results indicate that features formed using an adaptable H-PDLC mask have comparable aspect ratios to features fabricated using a binary mask. H-PDLC is a polymeric material formed holographically to have periodically spaced stratified layers of cured monomer and liquid crystal droplets. Reflection of a particular band of wavelengths occurs due to the periodicity of the layers and the index mismatch of the randomly aligned liquid crystal droplets. Bias applied to the film electrically aligns the liquid crystal layers eliminating the index mismatch yielding a transparent film.

1:51PM Q35.00012 Characterization of surface and pore morphologies on nanoporous organosilicate films...JEEUN KIM, HEEJU LEE, SANGHOON SONG, WONSUK CHA, HYUNJUNG KIM, GUNWOO PARK, SUNGKYU MIN, TAEHON LEE, HEEWOO RHEE, Sogang University, Korea, GWANGWOO KIM, Pohang Light Source Pohang, Korea — We have fabricated nanoporous organosilicate films with reactive porous trimethoxysilyl-propyl-cyclodextrin(TMSCD). With same amount of porogen loading, the films with reactive porogen TMSCD have shown higher mechanical strength than with those other non-reactive porogen. We have measured the pore morphologies depending on the types of porogens and loading densities along the pore generation processes by the grazing incidence small angle x-ray scattering, x-ray reflectivity, and ellipsometry. We measured the porosity of the film as a function of time and the annealing condition. We determined the actual porosity by measuring electron density of the films. In low loading density (10%~20%) porosity is very small and porosity distribution is uniform. In high loading density (>50%) the pores start to aggregate. We found that the porosity of the films can be affected easily by moisture. The results will be discussed with the mechanical properties along the optimized conditions for the films with ultra low dielectric constant.

2:03PM Q35.00013 Trap densities in porous low-k dielectric thin films as determined by optical and electrical measurements, J. JOANNA ATKIN, DAOHUA SONG, ROBERT LAIBOWITZ, Columbia University, EDUARD CARTIER, THOMAS SHAW, IBM Yorktown Heights, TONY HEINZ, Columbia University — Low-k dielectric materials based on porous carbon-doped oxides (p-CDOs), with relative dielectric constants as low as k = 2.1, are of great interest in the microelectronics industry. Knowledge of their basic electronic properties, such as energy gaps, barrier heights, and trap states, is essential for developing an understanding of their electrical leakage and stability characteristics. In particular, conduction via traps is a dominant mechanism in N$_2$ ambient stress of p-CDOs. We have fabricated porous organosilicate films with reactive porogen TMSCD with same amount of porogen loading. The techniques used include photoinduced current transients, optical second-harmonic generation measurements, and C-V electrical characterization. The low-k materials are shown to have relatively high trap densities (as compared with silicon dioxide films). The different behavior of bulk and interface traps will be discussed, along with the effects of annealing in various ambients.

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q36 GIMS: Focus Session: Advances in Scanned Probe Microscopy III: Force Methods
Morial Convention Center 228

11:15AM Q36.00001 Three-Dimensional Force Imaging and Quantification with Atomic Resolution...UDDO D. SCHWARCH, Department of Mechanical Engineering, Yale University — Atomic resolution images in noncontact atomic force microscopy (NC-AFM) reflect planes of constant frequency shift. To draw conclusions on the chemical activity at specific surface sites, however, the force acting between tip and sample should be known locally rather than the frequency shift. This is not an easy translation due to the non-linear nature of the relationship between the two. To overcome this problem, several groups have developed an extension to NC-AFM, dynamic force spectroscopy, which allows the precise, distance-dependent measurement of tip-sample forces. The forces are determined from frequency shift versus distance curves by mathematical analysis. Even though this approach had some success, prior attempts resulted either only in two-dimensional atomic resolution force xz-maps or in data sets of relatively low resolution, as long-term drift stability has been a problem. Using our recently completed home-built low temperature, ultrahigh vacuum NC-AFM, we were able to map the complete three-dimensional (3D) force field over a surface. Simultaneously, the tip-sample interaction potential and the energy dissipation of the oscillation process were recorded. As a test material, we used highly oriented pyrolitic graphite (HOPG) in order to study the atomic-scale origins of its qualities as a solid lubricant. Individual data points have been acquired over a surface area comprising several unit cells in a 3D grid with less than 6 pm grid size in all directions. From this data set, representations of cuts in any direction can be produced. While constant height images show atomic resolution with pN force resolution, vertical cuts visualize how the attractive force fields of the atoms extend into the vacuum space. We expect that the technique will find applications in fields of science where a local knowledge of interaction forces is beneficial, such as catalysis, chemical imaging, thin film growth, device fabrication, and tribology.
11:51AM Q36.00002 Tuning the instability in Static Mode Atomic Force Spectroscopy by applying electric field 1, SOMA DAS, S.N. Bose National Centre for Basic Sciences, P.A. SREERAM, Indian Institute for Science Education and Research, ARUP K. RAYCHAUDHURI, S.N. Bose National Centre for Basic Sciences — We study the force-distance (f-d) curves in the absence and presence of a dc bias between the cantilever tip and sample using Atomic Force Microscope (AFM). We find a new kind of bistability in the f-d curves obtained from Atomic Force Spectroscopy. The experimental signatures for this bistability point to a hysteresis like phenomenon when the f-d curves are cycled through the approach and retract paths. Interestingly, it is also observed that on application of a dc bias between the cantilever tip and sample, this bistability in the f-d curves can be tuned. This means that the “jump-into-contact” and “jump-off-contact” positions in the f-d curves change with the applied dc bias while keeping the other parameters constant. We simulate a simple model for AFM and show that this bistability is a characteristic feature of the experimental procedure and it can be controlled by applying a bias externally between the tip and sample.

1Financial support from DST is acknowledged

12:03PM Q36.00003 Theoretical simulation of tapping mode AFM in water, MASARU TSUKADA, Waseda University, NAOKI WATANABE, Mizuho Inf. & Res. Inst. — For the AFM of bio-molecules as proteins, the measurement in water is essential, since properties of bio-systems in vacuum are different from those in water. We developed a basic simulation method for the tapping mode AFM in water and applied to protein samples. First, the cantilever elastic body oscillation in water very close to the sample is analyzed, by solving the fluid dynamics of water simultaneously by a specially designed finite element method. The calculated resonance curve showed strong nonlinear features, as well as the reduction of resonant frequency and loss of the sharpness of the resonance. This method is useful for designing cantilever shapes. Next, the tapping process of the tip by the sample is simulated by a visco-elastic model of bio-samples obtained coarse graining the atomistic model. Sticking and detaching of the tip to the sample, which causes large disturbance of the cantilever motion, are also analyzed. With including these processes altogether, the frequency shift, dissipating energy, phase delay of the oscillation are obtained and used to calculate tapping mode images of proteins.

12:15PM Q36.00004 Functional probes for scanning probe microscopy, YUKIO HASEGAWA, Institute for Solid State Physics, The University of Tokyo, KOTONE AKIYAMA, Institute for Materials Research, Tohoku University, MASAYUKI HAMADA, TOYOAKI EGUCHI, TOSHU AN, Institute for Solid State Physics, The University of Tokyo, YASUNORI FUJIKAWA, TOSHIO SAKURAI, Institute for Materials Research, Tohoku University — In spite of importance of the probe in scanning probe microscopy (SPM), little attention was paid for the SPM probes for most of the measurements of SPM. We developed sharp metal-tip cantilevers with a typical curvature radius better than 5nm using focused ion beam (FIB) suitable for Kelvin probe force microscopy (KFM) 1. We obtained atomically resolved KFM images with an energy resolution less than 3meV with the probe 2. We also developed a glass-coated tungsten tip for synchrotron radiation-scanning tunneling microscopy with the FIB method 3 and obtained elementally resolved images in a resolution less than 20nm. We are now developing a precise atomic force microscope (AFM) lithography 4 with the FIB-milled tip attached to a quartz tuning fork controlled by non-contact AFM. We will present recent results of our AFM lithography such as an Au line with a width of 20~30 nm and characters drawn with Au nano dots on a Si surface. 1 K. Akiyama et al., RSI 76, 033705 (2005) 2 T. Eguchi, K. Akiyama et al., PRL 93, 266102 (2004) 3 K. Akiyama et al., RSI 76, 083711 (2005) 4 T. Eguchi, K. Akiyama et al., APL 89, 243119 (2006) 5 K. Akiyama et al., JP 61, 22 (2007).

12:27PM Q36.00005 Fabrication of a NEMS Resonator Over-shield for Mass Sensing, VINCENT T.K. SAUER, NINT, MARK R. FREEMAN, NINT and University of Alberta, WAYNE K. HIEBERT 1, NINT — The frequency shift of a resonating cantilever or bridge due to mass loading is dependent on the position of the loaded mass on the resonator. Therefore, for the purpose of accurate mass sensing, it is increasingly important to know the exact position of an added mass on a resonating mass sensor. Discussed is a novel technique to build over-shield structures on top of NEMS resonating devices to physically limit the position in which a loading mass can be deposited on a mass sensor. The over-shield is composed of a PECVD silicon nitride film which is supported by a sacrificial aluminum layer. Essentially, this MEMS over NEMS device acts as an integrated shadow mask for the resonator. With this over-shield device the effect of the position of added mass on a resonator is also examined.

1NINT is the National Institute for Nanotechnology, 11421 Saskatchewan Drive, Edmonton, AB, Canada, T6G 2M9

12:39PM Q36.00006 Ferromagnetic Resonance Investigation of an Individual Permalloy Dot Using Magnetic Resonance Force Microscopy, J. KIM, I.H. LEE, D. PELEKHOV, YU. OBUKHOV, P. BANERJEE, The Ohio State University, T. MARTIN, Los Alamos National Laboratory, P. WIGEN, P.C. HAMMEL, The Ohio State University — We report Ferromagnetic Resonance (FMR) investigations of individual 5.3 micron diameter permalloy dots using low temperature (4 K) Magnetic Resonance Force Microscopy (MRFM). The dot magnetization is saturated in the external magnetic field perpendicular to the plane of the sample. The evolution of the MRFM signal as probe-sample separation and the lateral probe position are varied reveals the shape of the magnetostatic modes excited in the dot in the presence of the strongly inhomogeneous magnetic field of the MRFM probe magnet. The experimental data agree excellently with micromagnetic modeling which suggests that localized FMR modes are excited in the sample. This effect opens the way for spatially resolved studies of ferromagnetic systems.

12:51PM Q36.00007 Detecting Few Electron Spins by Magnetic Resonance Force Microscopy with Potential Application for Donor Mapping in Semiconductor, KIN CHUNG FONG, PALASH BANERJEE, YURI OBUKHOV, DENIS PELEKHOV, P. CHRIS HAMMEL, Physics Department, Ohio State University — We report measurements of the statistical polarization of small electron spin ensembles by Magnetic Resonance Force Microscopy (MRFM). The experiments were conducted at T = 4 K using an IBM-style ultrasoft micromechanical cantilever outfitted with a high coercivity micromagnetic probe. Magnetic resonance signals from tens of electron spins with spin-correlation time of ~400 ns are obtained. In order to apply MRFM for spatial mapping of donor electrons in semiconductors, non-contact friction between the cantilever and the silicon surface is investigated. We found the combination of hydrogen passivation, gold coating, and shielding the sample surface from stray laser light reduces the non-contact friction by almost a factor of 100.

1:03PM Q36.00008 Force detected electron spin resonance from N@C₆₀ thin films, PALASH BANERJEE, K.C. FONG, D.V. PELEKHOV, P.C. HAMMEL, Dept of Physics, Ohio State University, Columbus OH 43210 — We report on force-detected electron spin resonance studies of thin films of endohedral fullerenes N@C₆₀. The electron spin associated with the nitrogen atom exhibits long spin-lattice relaxation times (T₁) at low temperatures. By combining microwave pulses with periodic adiabatic spin inversions in large gradients, we are able to selectively manipulate and detect the spins in submicron volumes. We also discuss our progress in detecting statistical fluctuations of the spin magnetization in this system using ultrasensitive force detection techniques.
1:15PM Q36.00009 Development of a $^3$He Nuclear Magnetic Resonance Force Microscope*, MARK MONTI, HAN-JONG CHIA, YONG LEE, JOHN MARKERT, Department of Physics, University of Texas at Austin — We report on construction of a $^3$He Nuclear Magnetic Resonance Force Microscopy (NMRFM) probe for nanoscale scanning and relaxation-time applications. Dual 3-axis piezo-driven stages yielded nanoscale positioning precision across several millimeters. We performed measurements on $^1$H nuclei in single crystal (NH$_4$)$_2$SO$_4$ in a sample-on-oscillator configuration at room temperature. A 0.25-mm-diameter permalloy magnet provided a field gradient of $\sim$500 T/m. The magnet position was scanned to achieve resonance; the RF frequency was also independently varied to verify the NMR nature of the force-detected signal. These first tests used a commercial AFM cantilever with a loaded resonance frequency of 2.0 kHz and spring constant of $\sim$0.03 N/m; motion was detected with a laser interferometer (1310 nm). Using cyclic adiabatic inversion (CAI), we detected a nuclear moment of $1.9 \times 10^{10}$ J/T with SNR $\approx 6$. By preceding the CAI sequence with a short, variable-length pulse, a spin-nutation signal was observed over several cycles of period 17 $\mu$s, implying a rotating RF field of 14 G. Using a $(\pi/2)$-r-$(\pi/2)$-CAI sequence, a spin-echo was mapped out, with a FWHM of 8 $\mu$s. We also discuss plans to extend measurements towards the base temperature of the probe, 0.3 K. *This work was supported by NSF Grant Nos. DMR-0605828 and DGE-0549417.

1:27PM Q36.00010 NMR Force Microscopy on Co/Cu interface , YU. OBUKHOV, D. V. PELEKHOV, P. BANERJEE, J. MARTINDALE, K. C. FONG, P. C. HAMMEL — We present our recent NMR Force Microscopy experiments, where we demonstrate the first detection of 63Cu and 65Cu NMR using Magnetic Resonance Force Microscopy (MRFM). The signals were detected at T = 5 K using a commercial Si3N4 cantilever with a spherical NdFeB probe magnet. We demonstrate MRFM detection sensitivity of 1.0e5 nuclear spins. We report measurements of the relaxation time, signal lifetime, and the results of nutation experiments. We also discuss the application of MRFM for spatially resolved mapping of the local hyperfine field variation in the vicinity of a buried Co/Cu interface arising from the RKKY interaction.

1:39PM Q36.00011 Micromagnetic Modeling of Localized Ferromagnetic Resonance Detected with Magnetic Resonance Force Microscopy, DENIS V. PELEKHOV, Ohio State University, IVAR MARTIN, Los Alamos National Laboratory, YURI OBUKHOV, JONGJOO KIM, INHEE LEE, Ohio State University, EVGUENI NAZARETSKI, ROMAN MOVSHOVICH, Los Alamos National Laboratory, P. CHRIS HAMMEL, Ohio State University — Magnetic Resonance Force Microscopy (MRFM) is a novel scanned probe technique based on mechanical detection of magnetic resonance. Its extreme sensitivity originates partially from the high magnetic field gradient of MRFM probe micromagnet which couples the MRFM probe to the magnetic moments in the sample. We report micromagnetic modeling of Ferromagnetic Resonance (FMR) performed in the local field of the micromagnetic MRFM probe: its strongly inhomogeneous field enables the excitation of localized FMR modes in the sample. This unusual effect provides a mechanism for spatially resolved FMR investigations of ferromagnetic systems. We discuss spatial resolution and results for both quasi 2D and 1D systems.

1:51PM Q36.00012 Magnetic Resonance Force Microscopy System Design for the Study of Organic Materials, DORAN SMITH, US Army Research Laboratory — We will present an overview of our program to study organic materials with MRFM.

2:03PM Q36.00013 Applications of scanning Kelvin probe microscopy in the characterization of photovoltaic materials and devices, CHUNSHENG JIANG, HELIO MOUTINHO, MOIMAF Ak-JASSIM, NATIONAL RENEWABLE ENERGY LABORATORY TEAM — We have in recent years developed scanning Kelvin probe microscopy (SKPM), and applied this nanometer resolution technique to the characterization of III-V, II-VI, and thin film Si-based single- and multi-junction solar cell devices. In this presentation, we will report our improvements of the SKPM technique and show three examples of the potential measurements. We will first show a Bi-incorporation-induced junction movement in a MBE-grown single-junction GaInNAs cell. This junction movement caused significant device degradation, especially in the short wavelength range. We then present potential distributions among the top and bottom junctions in a GaInP$_2$/GaAs tandem-junction cell. A light-induced potential flattening in the top junction and a potential accumulation in the bottom junction was clearly measured. Lastly, we will show a non-uniform distribution of the electric field across an a-Si:H $n$−$i$−$p$ junction, and this electric field was significantly improved by depositing buffer layers at the $n/i$ and $i/p$ interfaces.

Wednesday, March 12, 2008 11:15AM - 2:15PM –
Session Q37 FIAP: Magnetotransport in 2DEGs Morial Convention Center 229

11:15AM Q37.00001 Effective mass suppression in interacting, fully spin-polarized 2D electron systems in wide A1As quantum wells , MEDINI PADMANABHAN, T. GOKMEN, N.C. BISHOP, M. SHAYEGAN, Dept. of Electrical Engineering, Princeton University — We report effective mass measurements, via analyzing the temperature dependence of the Shubnikov-de Haas oscillations, in dilute two-dimensional electron systems (2DEGs) confined to wide A1As quantum wells. In this system electrons have an anisotropic in-plane Fermi contour. When the 2DEG is partially spin-polarized, the effective mass is larger than its band value and increases as the density is reduced, consistent with previous results in various 2DEGs. An unexpected trend emerges as we fully spin-polarize the 2DEG by subjecting it to a strong parallel magnetic field: the mass falls below the band value and tends to decrease with decreasing density.

11:27AM Q37.00002 Effective mass suppression in interacting, fully spin-polarized 2D electron systems in narrow A1As quantum wells , TAYFUN GOKMEN, MEDINI PADMANABHAN, K. VAIKILI, M. SHAYEGAN, Department of Electrical Engineering, Princeton University — Similar to the study described by M. Padmanabhan et al. (previous abstract), we perform effective mass measurements in a two-dimensional electron system (2DEG) confined to a narrow (45Å-wide) A1As quantum well. In contrast to the 2DEGs confined to wide A1As quantum wells, in this system the electrons occupy a single out-of-plane valley with an isotropic in-plane Fermi contour. We confirm that the effective mass for the fully spin-polarized 2DEG is suppressed compared to the partially spin-polarized value.
11:39AM Q37.00003 Effects of mass anisotropy, thickness and disorder on the spin susceptibility of the 2DEG in AlAs QWs. MARIAPA MARCHI, STEFANIA DE PALO, GAETANO SENATORE, Democritos IFNM-CN and Università di Trieste, SAVERIO MORONI, Democritos IFNM-CN and SISSA — We present predictions of the spin susceptibility $\chi^s$, obtained from extensive DMC simulations, for a two dimensional (2D) electron gas (EG) with mass anisotropy appropriate to AlAs QWs[1], both in the strictly 2D limit and with thickness included. We demonstrate that in the one-valley case anisotropy suppresses $\chi^s$ substantially at all densities and in particular at those relevant to experiments[1], the effect being larger at lower density. This suppression adds onto the one due to thickness[2,1]. The comparison of our results for a model EG including both thickness and anisotropy with experiments for AlAs QW’s[1] reveals the role of disorder in determining the measured spin susceptibility. In the two-valley case we find an interesting interplay of anisotropy and valley degree of freedom in determining the EG properties and in particular the spin susceptibility. [1] T. Gokmen et. al., Phys. Rev. B in press and cond-mat 0711.1294. [2] S. De Palo et. al., Phys. Rev. Lett. 94, 226405 (2005); and to be published.

11:51AM Q37.00004 Heat Transport Measurements on 2D Electron Systems at Zero Magnetic Field using Quantum Points Contacts. D.A. NICHOLS, G. GRANGER, J.P. EISENSTEIN, Caltech, J.L. RENO, Sandia, L.N. PFEIFFER, K.W. WEST, Bell Labs — Three adjacent quantum point contacts (QPCs) separated by 20 micrometers are fabricated along the edge of a GaAs/AlGaAs two-dimensional electron gas (2DEG). The 2DEG is heated locally by passing an alternating current through the middle QPC, which is tuned so only a few channels propagate. A thermovoltage develops across a detector QPC on either side of the heater, and its gate voltage dependence is related to the derivative of the conductance of the detector QPC as expected from Mott’s formula. The thermovoltage depends on power and temperature and are also investigated. These experiments illustrate the feasibility of using mesoscopic devices to study heat transport in 2D electron gases with various geometries.

This work was supported by Microsoft Research Project Q.

12:03PM Q37.00005 Observation of Chiral Heat Transport in the Quantum Hall Regime. G. GRANGER, D.A. NICHOLS, J.P. EISENSTEIN, Caltech, J.L. RENO, Sandia, L.N. PFEIFFER, K.W. WEST, Bell Labs — The nature and properties of heat transport at the edge of a quantum Hall state are investigated using three adjacent quantum point contacts (QPCs) separated by 20 micrometers fabricated along the edge of a GaAs/AlGaAs two-dimensional electron gas (2DEG). With the bulk of the device at filling factor $\nu=1$, a thermovoltage signal appears across a detector QPC only on one side of the heater QPC depending on the direction of the magnetic field. This behavior indicates that heat transport is chiral at this filling factor. Raising the temperature decreases the thermovoltage, as the electrons carrying the heat find more ways to cool off at higher temperatures. When the distance between the heater and the detector is doubled, the thermovoltage is reduced, meaning that the electrons cool significantly over distances on the order of tens of micrometers. These findings are qualitatively insensitive to the exact magnetic field over the field range corresponding to the $\nu=1$ minimum.

This work was supported by Microsoft Research Project Q.

12:15PM Q37.00006 Momentum resolved transport spectroscopy of quantum Hall edges in a bent quantum well. LUCIA STEINKE, A. FONTCUBERTA I MORRAL, M. BICHLER, G. ABSTREITER, Tech. Univ. Muenchen, M. GRAYSON, Northwestern University — A new magnetic field orientation is introduced for a bent quantum well, such that momentum-resolved edge-state spectroscopy is possible up to fractional filling factors. A bent quantum well (BQW) provides a unique way of coupling to quantum Hall edges when the junction length is reduced to the mean free path $\sim 10\mu m$, constituting a weak link between the two facets. With a magnetic field $B$ perpendicular to one facet, the other facet can probe momentum-resolved transport spectroscopy of the edge states even though no barrier is present. We measure the differential conductance $dI/dV$ across the BQW as a function of the dc bias voltage $V_d$ at fields below 3 T and $\nu < 1/3$. Above $1.5 T$ a conductance-suppression gap develops around zero bias, and resonance peaks are observed at the gap edges, reminiscent of previous momentum-resolved work. The gap size increases and at $6 T$ becomes asymmetric, with one of the flanking resonances becoming stationary and extremely sharp. These main features can be interpreted in terms of momentum resolved coupling, and the positions of these features are in good quantitative agreement with Hartree calculations of this system.

Supported by DFG GR-2618/1-1, work performed at NHMFL.

12:27PM Q37.00007 From insulating behavior to quantum Hall liquid at low magnetic fields. T.-Y. HUANG, CHI-TE LIANG, National Taiwan University, GIL-HO KIM, Sungkyunkwan University, CHUN FENG HUANG, CMS/NML, ITRI, C.-P. HUANG, J.-Y. LIN, H.-S. GOAN, National Taiwan University, D.A. RITCHIE, Cambridge University — It is an interesting, but unsettled issue whether a direct transition from an insulating (I) state to a quantum Hall (QH) liquid is a genuine phase transition where $\nu$ denotes the filling factor [1]. It is argued that the observed low-field direct transition is not a quantum phase transition, but can be ascribed to a crossover from weak localization to Landau quantization (LQ) [1]. We shall show that between the insulating region and the QH regime, multiple temperature (T)-independent points in the longitudinal resistance can be observed in a moderate-mobility two-dimensional electron system containing InAs quantum dots. Interestingly, the amplitudes of the accompanying resistance oscillations can be well approximated by the conventional Shubnikov-de Haas theory, suggesting metallic behavior. Moreover, our data show that LQ can modulate the density of states without causing the formation of a QH liquid, demonstrating that the crossover from insulating behavior to Landau quantization can occur over a wide range of magnetic field. We speculate that to obtain a correct insight into the low-field I-QH transition, the argument raised by Huckestein [1] ought to be modified. Ref: [1] B. Huckestein, PRL 84, 3141 (2000) and references therein.

12:39PM Q37.00008 In-plane field induced anisotropy in the microwave/rf resonances of 2D electrons at the second excited Landau level. HAN ZHU, Princeton Physics, G. SAMBANDAMURTHY, SUNY Buffalo, L. ENGEL, NHMFL/FSU, D. C. TSUI, Princeton EE, L. PFEIFFER, K. WEST, The Bell Labs, Alcatel-Lucent Technologies — We report measurements of the microwave/rf diagonal conductivity of ultrahigh mobility 2D electron systems in GaAs/AlGaAs quantum wells, at the second excited Landau level (LL), with in-plane magnetic field $B_{ip}$. Previous measurements [1] at $B_{ip} = 0$ have found an essentially isotropic pinning mode resonance of the bubble phase near LL filling $4.15$ to $4.4$. As $B_{ip}$ is applied, with the rf electric field $E$ either parallel or perpendicular to $B_{ip}$, the peak frequencies $f_{pk}$ and resonance widths almost identically increase, probably due to stronger pinning as the electron wavefunction is being pushed closer to the GaAs/AlGaAs interface. However, $B_{ip}$ is found to induce anisotropy in the ratio of the integrated intensity $S$ over $f_{pk}$, which is thought to be proportional to the participating carrier density. As $B_{ip}$ is applied, $S/f_{pk}$ increases with $E$ perpendicular to $B_{ip}$, and decreases with them parallel. Similar behavior is found in the resonances from the Wigner crystal phase formed with the same LL. [1] R. Lewis et al., PRL 89,136804 (2002).
12:51PM Q37.00009 Microwave modes of two dimensional electron systems near macroscopic ferromagnets
1. BRENDEN MAGILL, NHMFL and MARTECH, FSU. L. W. ENGEL, NHMFL/FSU, M. P. LILLY, J. A. SIMMONS, J. L. RENO, Sandia National Laboratory — We report on microwave measurements of a high mobility two dimensional electron system (2DES) in a homogeneous external field \( B_0 \), and with cylindrical ferromagnets of radii \( r_m \) placed on the surface of the sample with the long axis perpendicular to the 2DES. The magnet materials are Dy and permalloy, and \( r_m \) varies from 0.5 mm to 0.125 mm. Microwave spectra measured for transmission between two ohmic contacts show resonant absorption at peak frequency, \( f_{pk} \), decreasing as \( B_0 \) or \( r_m \) increase. We will interpret the data in terms of plasma excitations similar to edge magnetoplasmoids [1] confined under the edges of the magnets by the large magnetic field gradients there. [1] See, for example, V. A. Volkov and S. A. Mikhailov, Sov. Phys.-JETP 67, 1639 (1988).

3 This work supported by MARTECH

1:03PM Q37.00010 Radiation-induced decay of Shubnikov-de Haas oscillations in the regime of the radiation-induced zero-resistance states in GaAs/AlGaAs devices.

1:15PM Q37.00011 Floquet Theory of Magneto-Resistance Oscillations in Microwave Irradiated 2DEGs.
ASSA AUERBACH, G. VENKETESWARA PAI, Physics Department, Technion — Some remarkable phenomena have been recently observed in semiconductor heterostructures: microwave induced resistivity oscillations (MIRO), Hall induced resistivity oscillations (HIRO), and zero resistance states (ZRS). These effects were seen at weak magnetic fields and high temperatures, where Shubnikov-de-Hass oscillations are thermally smeared and the transport is expected to be classical Drude-like. However microwave radiation, or large Hall currents expose the underlying Landau quantization and result in MIRO and HIRO. Theoretically, it is essential to get the full nonlinear current-field response in the presence of strong radiation fields and disorder to handle these effects. Here we generalize the Floquet operator approach to incorporate arbitrary large electric fields into the zeroth order evolution operator. We construct the disordered Floquet evolution operator which allows us to systematically calculate the nonlinear photocurrent to second order in short range disorder. We derive the magnitude of MIRO from the microscopic parameters. We deduce the optimal conditions for observing large MIRO and ZRS effects. We determine the characteristic Hall fields clarifying the HIRO, and the magnitude of spontaneous ZRS fields. Reference: A. Auerbach and G. V. Pai, Phys. Rev. B 76, 205318 (2007).

1:27PM Q37.00012 The origin of the stripes observed in scanning single-electron transistor and in mesoscopic transport measurements of quantum Hall samples
CHENGGANG ZHOU, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, MONA BERCIOU, Department of Physics and Astronomy, University of British Columbia — We analyze two seemingly unrelated types of experiments on quantum Hall samples. When the measured quantities (local compressibility and resistances) are plotted as a function of magnetic field (\( B \)) and electron density (\( n_e \)), both experiments exhibit stripes parallel to lines of integer filling factors on the \( B-n_e \) plane. Unlike the popular belief in Coulomb blockade physics, we explain this within the framework of non-interacting electron theory. Our numerical simulations and theoretical analysis demonstrate that new electronic states appear predominantly at the center of Landau levels, when the magnetic field increases. This leads to a certain “spectral ordering” of the localized states that is sufficient to explain the main features observed in the experiments.

1:39PM Q37.00013 External Field Effecting Excitonic Superfluid in Drag Geometry.
JUNG-JUNG SU, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin — We will report on transport properties of excitonic superfluid under the influence of external applied field in generalized drag geometries. In such geometry, voltages are applied to the driven layer and a tunnable load resistance is added across the drag layer, which enable current flows in the drag layer when an excitonic condensate is established. The physics of the excitonic superfluid is described macroscopically by classical model and justified by microscopic mean-field plus non-equilibrium Green’s function (NEGF) approach. We found that the excitonic superfluid only exist in the voltage configurations in which charge conservation law is satisfied, given a zero tunneling system. This system is then well described by a set of circuit, on the premise that the quasiparticle current can not flow through the system, and the current thus obtained is in great consistence with our NEGF calculation. Finally, we proposed a method of detecting tunneling strength by the non-conservation of charge in the presence of bare tunneling.

1:51PM Q37.00014 Supersolid of indirect excitons in electron-hole quantum Hall systems.
CHANG-HUA ZHANG, YOGESH N. JOGLEKAR, Indiana University—Purdue University Indianapolis — We investigate the ground state of a balanced electron-hole system in the quantum Hall regime using mean-field theory and obtain its phase diagram as a function of interlayer distance \( d \) and the filling factor within a layer. We identify an excitonic condensate phase, a supersolid phase, as well as uncorrelated Wigner crystal states. We find that balanced electron-hole system exhibits a supersolid ground state over a wide range of the filling factors. We obtain the ground state stiffness in the the excitonic phases and show that the phase transitions from a uniform condensate to a supersolid is accompanied by a marked change in the stiffness. Our results provide the first semi-quantitative determination and analysis of the supersolid of excitons.

2:03PM Q37.00015 Insulating, Metallic, and Superconducting Transport regimes of 2D Amorphous Superconducting Films in B-T-Disorder Space.
YIZE LI, JONGSOO YOON, University of Virginia — Amorphous tantalum thin films are known to exhibit a superconductor-metal-insulator transition in the zero temperature limit with increasing magnetic fields. The metallic phase intervening the superconducting and insulating phase is unexpected. Each phase is known to exhibit unique nonlinear transport properties[1] with intrinsic origins[2]. In order to study how the mechanism behind each phase is influenced by B, T, and disorder, we have measured the evolution of nonlinear transport properties by changing B, T, and disorder. The resulting “phase diagram” of a sample with normal state sheet resistivity of 2.3 kilo-ohm indicates that the superconducting phase is completely surrounded by metallic phase, and a direct superconductor-insulator transition is not allowed. Recently, we extend our study on other samples with different disorder that is controlled by film thickness. By combining these results, we can map out the 3D phase diagram in B-T-disorder space. [1] Y. Qin et al., Phys. Rev. B 73, 100505(R) (2006). [2] Y. Seo et al., Phys. Rev. Lett. 97, 057005 (2006).
11:51AM Q38.00002 Intrinsic Bipolar Carrier (e⁻/h⁺) Layer on Clean Surface of Insulating BaTiO₃, Y. WATANABE, D. MATSUMOTO, Y. URAKAMI, S. KAKU, Kyushu U, Japan — We show experimentally the electron/hole layer on the clean surface of insulating pure BaTiO₃ single crystals in ultra high vacuum, which is the first report of the bipolar surface carrier layer by the field effect on any oxide to our knowledge. The experiments here demonstrate that the surface carrier layer is not due to impurities or defects but is intrinsic due to the spontaneous polarization P₀. The surface carrier layer induced by P₀ was found to exist at least to 80K on atomically ordered surface of insulating BaTiO₃, which has become the basis of a recent new memory device. However, much skepticism about its intrinsic nature is unresolved. We report here the disappearance of the carrier layer above Curie temperature, its disappearance by the exposure to a low vacuum, which indicates its location as the top surface, and, both electron/hole carrier layers by P₀. Here, the control of the electron and hole surface layer is only through the direction of poling. The realization of the hole layer is clear evidence that oxygen vacancies are inessential to the formation of the carrier layer, because oxygen vacancies kill the hole carrier layers. The present results have various implications for the basis of ferroelectric materials such as nano-ferroelectrics, field effects and domains. “Watanabe et al., Phys. Rev. Lett. 86, 332 (2001).”

12:03PM Q38.00003 Contrast in ultrathin film ferroelectric behavior between air and vacuum environments, A. P. BADDORF, P. MAKSYMOWYCH, S. V. KALININ, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, R. RAMESH, Department of Materials Science, University of California, Berkeley — At nanoscale dimensions, ferroelectric properties of oxide materials are dominated by depolarizing effects which depend strongly on the electrostatic screening at the interfaces and the environment. Oxide surfaces readily react with adsorbed molecules that may chemically or electronically alter the ferroelectric behavior. We have examined ultrathin (5-20 nm) BiFeO₃ thin films grown on SrTiO₃(110) using ultra-high vacuum Piezoresponse Force Microscopy. All the films reveal a characteristic behavior trend that in air the films are uniformly polarized, while multiple domains are observed in vacuum. The monodomain to polydomain transition occurs via either annealing in oxygen or simple evaporation, which suggests that mole fraction of oxygen on the surface. Local ferroelectric switching behavior has also been compared for vacuum and ambient environments on the same substrate. Measurements were made at the Center for Nanophase Materials Sciences, sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. DOE.

12:15PM Q38.00004 X-ray Studies of Chemical Switching of PbTiO₃ on SrRuO₃, CAROL THOMPSON, Dept. of Physics, Northern Illinois Univ., R.-V. WANG, D.D. FONG, F. JIANG, S.K. STREIFFER, P.H. FUOSS, J.A. EASTMAN, G.B. STEPHENSON, Argonne National Laboratory — Recent studies have shown that monodomain polarization can be stabilized in thin films not only through the presence of electrodes that provide electronic compensation at the film interfaces but also through surface-adsorbed ions or charged interfacial defects/impurities. Here, we use real-time synchrotron x-ray scattering to investigate changes in the polarization of PbTiO₃ films induced by varying the chemistry of the vapor above the film surface. We observe the sign of the polarization can be reversibly switched by changing the partial pressure of oxygen (pO₂) in equilibrium with the film surface. The dependence of film lattice parameter on pO₂ is bistable, following a butterfly loop analogous to that observed under applied voltage. The large compressive strains observed in the thinnest films prior to switching indicate that the chemical switching process can result in electric fields approaching the intrinsic coercive field for PbTiO₃. Work supported by the U. S. Department of Energy under Contract No. DE-AC02-06CH11357.

12:27PM Q38.00005 First-principles prediction of switchable stoichiometry at interfaces, SERGEY V. LEVCHENKO, ANDREW M. RAPPE, University of Pennsylvania — We present a first-principles density functional theory (DFT) study of the relative thermodynamic stability of ferroelectric (FE) lithium niobate (LiNbO₃) (0001) surfaces of different stoichiometry. We predict that the equilibrium stoichiometries are different for the positively and negatively polarized LiNbO₃ surfaces under the same conditions. A correct way of calculating surface charges for ferroelectric materials with intrinsic polar stacking is developed. It is found that surface charge passivation by ions is thermodynamically favored over passivation by mobile carriers in a wide range of chemical potentials.

12:39PM Q38.00006 Phase Field Modeling of Ferroelectric Thin Films with Space Charge, RAJEEV AHLUWALIA, Instute of Materials Research & Engineering, Singapore, NATHANIEL NG, Institute of High Performance Computing, Singapore, HAIBIN SU, FREDDY BOEY, Nanyang Technological University, Singapore — The time-dependent Ginzburg-Landau (TDGL) equations and phase field modeling have been used to describe various phenomena in ferroelectric materials, such as domain nucleation and evolution, and hysteresis. This work applies the TDGL model to explain the behavior of perovskite ferroelectric thin film with space charge. Results show that the presence of space charge at the surface significantly influences the switching process and domain structures in ferroelectric thin films. The role of space charge on size effects is also studied.
12:51PM Q38.00007 One-dimensional polydomains in Ferroelectric thin films, MATIAS NUNEZ, North Carolina State University, MARCO BUONGIORNO NARDELLI, North Carolina State University — The local nature of the interface in metal/ferroelectric oxide junctions can drastically affect the polarization in the ferroelectric film. As the thickness of the film is reduced, the intensity of the depolarization field increases and the system will reduce its electrostatic energy in two ways, either by forming lateral 180° domains [1], or by reducing the ionic polarization while remaining in a monodomain state. Using DFT, maximally localized Wannier functions [2] and the layer polarization concept [3], we studied the ferroelectricity in thin layers of BaTiO$_3$ sandwiched between metal. Our results suggest that the structures associated with this spatial scale are more complex than previously thought, and we show how a pattern of the local polarization provides another way to minimize the internal energy below certain critical thickness. This pattern is characterized by the appearance of one-dimensional polydomains, consecutive dipoles with opposed orientations in the direction perpendicular to the ferroelectric thin film/metal interface.


1:03PM Q38.00008 Theory of Electric Polarization Induced by Inhomogeneity in Crystals, DI XIAO, The University of Texas at Austin, JUNREN SHI, Institute of Physics, Chinese Academy of Sciences, DENNIS CLOUGHERTY, The University of Vermont, QIAN NIU, The University of Texas at Austin — We develop a general theory of electric polarization induced by inhomogeneity in crystals. We show that contributions to polarization can be classified in powers of the gradient of the order parameter. The zeroth order contribution reduces to the well-known result obtained by King-Smith and Vanderbilt for uniform systems. The first order contribution, when expressed in a two-point formula, takes the Chern-Simons 3-form of the vector potentials derived from the Bloch wave functions. Using the relation between polarization and charge density, we demonstrate our formula by studying charge fractionalization in a two-dimensional dimer model recently proposed.

1:15PM Q38.00009 Ferroelectric Thin Films Under Inhomogeneous Electric Fields - Lateral Size and Thickness Dependence, NATHANIEL NG, Institute of High Performance Computing, Singapore, RAJEEV AHLUWALIA, Institute of Materials Research & Engineering, Singapore, HAIBIN SU, FREDDY BOEY, Nanyang Technological University, Singapore — Advances in nanoscale ferroelectric devices have led to interest in studying size effects in ultrathin films whose properties differ substantially from the bulk. We present our results from ferroelectric thin films on SrRuO$_3$/SrTiO$_3$ substrate for onset of (meta)stable memory should be in excess of 4.5 nm compared with critical thickness of 1.6 nm for existence of ferroelectric domains.

1:39PM Q38.00011 Transport properties of epitaxial ferroelectric trilayer heterostructures with BaTiO$_3$ barriers, D.A. FELKER, H.W. JANG, C.B. EOM, M.S. RZCHOWSKI, University of Wisconsin-Madison — We studied the influence of the polarization on the transport properties of epitaxial trilayer heterostructures with SrRuO$_3$ metallic oxide electrodes and ferroelectric BaTiO$_3$ barriers. The heterostructures were grown using atomic-layer controlled pulsed laser deposition, with barrier thickness ranging from 4 nm to 100 nm. We discuss the frequency and thickness dependence of the P-E loops, and both voltage-biased and current-biased current-voltage (I-V) characteristics. We find that the I-V curves of the thinnest barriers show a hysteresis due to the switching of the polarization in the ferroelectric barrier, leading to a change in the conductance of the junction. A ferroelectric junction with clear resistive switching is a candidate for nonvolatile memory applications.

1:51PM Q38.00012 $^{17}$O Nuclear Magnetic Resonance Chemical Shielding Calculations of PZT Solid Solutions, DANIEL L. PECHKIS, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — First principles B3LYP calculations of $^{17}$O NMR in PbTiO$_3$, Pb(Zr$_{0.55}$Ti$_{0.45}$)$_3$O$_5$ (PZT), and PbZrO$_3$ will be presented. These systems were modeled with finite size quantum clusters embedded in point charge arrays. The embedding reproduces the Ewald Coulomb potential to better simulate the crystal environment. For polar systems, the calculations were performed in the presence of an external electric field to cancel surface depolarization effects. PZT was modeled using three chemically ordered structures: P4mm, P2mm, and R3m. Two groupings of $^{17}$O isotropic chemical shifts $\delta_{iso}$ are seen in all of our PZT calculations with [001] ordering. One is at $\delta_{iso}$ ≈ 400ppm and the other is at $\delta_{iso}$ ≈ 650ppm. We relate these to variations in the Ti-O and Zr-O bond lengths and use this to interpret recent experimental measurements.

2:03PM Q38.00013 First-principles calculation of phonon dispersions for Ba$_{1-x}$Ca$_x$TiO$_3$, TAICHI KOSUGI, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo — Amongst perovskite oxides, BaTiO$_3$(BTO) is widely used for its distinct dielectric, piezoelectric and optical properties. Its lattice dynamics, associated with atomic displacements, have been intensively studied both theoretically and experimentally, since it is essential for the dielectric instability of this material. Recently Ca-doped BTO(BCTO) single crystal was synthesized by Fu et al. and found to have exotic natures. Using the direct method proposed by Parlinski, we calculated the phonon dispersions of BCTO in a fully ab initio manner, in which the force constants, the Born effective charges and the dielectric tensors are determined from first-principles.

1Supported by ONR
2Supported by Virginia Space Grant Consortium Fellowship
4S. Li and K. Rabe. APS March Meeting abstract (2007).

This work was supported by the Next Generation Super Computing Project, Nanoscience Program, MEXT, Japan.
11:15AM Q39.00001 Self-Organized Porous Nanostructures in Anodized Metal Oxide, LIAM STANTON, ALEXANDER GOLOVIN, Northwestern University — We consider the self-organization of porous nanostructures in anodized metal oxide. We have developed a mathematical model which incorporates the electro-chemical transport of oxygen anions within the oxide layer and the chemical reactions at the metal-oxide and oxide-electrolyte interfaces. It is shown through linear stability analysis, that a short-wave instability exists in certain parameter regimes which leads to the formation of hexagonally ordered pores observed in anodized aluminum oxide. Numerical simulations validate these results.

11:27AM Q39.00002 Intercalation of Li Ions into a Graphite Anode Material: Molecular Dynamics Simulations, IBRAHIM ABOU HAMAD, HPC², Mississippi State University, MARK NOVOTNY, HPC² and Department of Physics and Astronomy, Mississippi State University — Large-scale molecular dynamics simulations of the anode half-cell of a lithium-ion battery are presented. The model system is composed of an anode represented by a stack of graphite sheets, an electrolyte of ethylene carbonate and propylene carbonate molecules, and lithium and hexafluorophosphate ions. The simulations are done in the NVT ensemble and at room temperature. One charging scheme explored is normal charging in which intercalation is enhanced by electric charges on the graphitic sheets. The second charging mechanism has an external applied oscillatory electric field of amplitude A and frequency f. The simulations were performed on 2.6 GHz Opteron processors, using 160 processors at a time. Our simulation results show an improvement in the intercalation time of the lithium ions for the second charging mechanism. The dependence of the intercalation time on A and f will be discussed.

11:39AM Q39.00003 Aging processes in reversible diffusion-limited reactions, VLAD ELGART, MICHEL PLEIMLING, Virginia Polytechnic Institute and State University — Reversible diffusion-limited reactions display anomalous (i.e. slow) dynamics characterized by a power-law relaxation toward stationarity. In contrast to previous studies that focused on the time-dependence of this relaxation, we study here the nonequilibrium behavior of various simple reversible reaction-diffusion models in the aging regime. Starting from the exact Langevin equations describing these models, we derive expressions for two-time autocorrelation and autoresponse functions and obtain a simple aging behavior for these quantities. The autoresponse function is thereby found to depend on the specific nature of the chosen perturbation of the system.

11:51AM Q39.00004 Lyapunov modes in coupled map lattices¹, GUENTER RADONS, HONGLIU YANG, Institute of Physics, Chemnitz University of Technology — Hydrodynamic Lyapunov modes, which have recently been observed in many extended systems with translational symmetry, such as hard sphere systems, dynamic XY-models, or Lennard-Jones fluids, are nowadays regarded as fundamental objects connecting Nonlinear Dynamics and Statistical Physics. A solution to one of the puzzles, the appearance of good and of “vague” modes, is presented here for the model system of coupled map lattices: The structural properties of these modes are related to the phase space geometry, especially the angles between Oseledec subspaces, and to fluctuations of local Lyapunov exponents. The numerical calculation of these quantities is achieved with the new algorithm proposed in [1]. In this context we report also on the possible appearance of branches in the Lyapunov spectra of inhomogeneous systems [2], similar to acoustic and optical branches for phonons. [1] F. Ginelli et al., PRL 99, 130601 (2007). [2] H. Yang and G. Radons, PRL 99, 164101 (2007)

¹Support from Deutsche Forschungsgemeinschaft and the John von Neumann Institute for Computing is gratefully acknowledged.

12:03PM Q39.00005 Simulation of nonlinear pattern formation dynamics in photoinduced structure change¹, KUNIO ISHIDA, Corporate R&D Center, Toshiba Corporation, Japan, KEIICHIRO NASU, Institute of Materials Structure Science, KEK, Japan — We study the nonlinear dynamics of pattern formation triggered by injection of photoexcited states. In order to describe the nonadiabatic relaxation during the relaxation process, we employ a model of localized electrons coupled with a fully quantized phonon mode, and the time-dependent Schrödinger equation for the model is numerically solved. We found that the photoinduced nucleation process is switched on only when certain amount of excitation energy is supplied in a narrow part of the system, i.e., there exists a smallest cluster of excited molecules which makes the nucleation possible. As a result, the portion of the cooperatively converted molecules is nonlinearly dependent on the photoexcitation strength, which has been observed in various materials.

¹This work was supported by the Next Generation Super Computing Project, Nanoscience Program, MEXT, Japan.

12:15PM Q39.00006 A study of some non-equilibrium driven models and their contribution to the understanding of molecular motors, IRINA MAZILU, JOSHUA GONZALEZ, Washington and Lee University — From the point of view of a physicist, a bio-molecular motor represents an interesting non-equilibrium system and it is directly amenable to an analysis using standard methods of non-equilibrium statistical physics. We conduct a rigorous Monte Carlo study of three different driven lattice gas models that retain the basic behavior of three types of cytoskeletal molecular motors. Our models incorporate novel features such as realistic dynamics rules and complex motor-motor interactions. We are interested to have a deeper understanding of how various parameters influence the macroscopic behavior of these systems, what is the density profile and if the system undergoes a phase transition. On the analytical front, we computed the steady-state probability distributions exactly for the one of the models using the matrix method that was established in 1993 by B. Derrida et al. We also explored the possible features offered by the “Bethe ansatz” method by mapping some well studied spin models into asymmetric simple exclusion models (already analyzed using computer simulations), and to use the results obtained for the spin models in finding an exact solution for our problem. We have exhaustive computational studies of the kinesin and dynein molecular motor models that prove to be very useful in checking our analytical work.

12:27PM Q39.00007 Controlling surface morphologies by time-delayed feedback¹, BEATE SCHMITTMANN, Virginia Tech, MICHAEL BLOCK, ECKHERD SCHOELL, Technische Universitaet Berlin — We propose a new method to control the roughness of a growing surface, via a time-delayed feedback scheme. The method is very general and can be applied to a wide range of non-equilibrium growth phenomena, from solid-state epitaxy to tumor growth. Possible experimental realizations are suggested. As an illustration, we consider the Kardar-Parisi-Zhang equation in 1+1 dimensions and show that the effective growth exponent of the surface width can be stabilized at any desired value in the interval [0.25,0.33], for a significant length of time.

¹We acknowledge partial support from the NSF through DMR 0414122 and the DPG through SFB 296.
12:39PM Q39.00008 Schwoinger-Keldysh Formalism for Non-Hermitian Quantum Problems: A Case Study on Non-Equilibrium Steady State Transport, PAATA KAKASHVILI, C.J. BOLECH, Physics and Astronomy Department, Rice University, Houston, TX 77005, USA — Non-unitary quantum mechanics has been used in the past to study irreversibility, dissipation and decay in a variety of physical systems. In this presentation, we propose a general scheme to deal with systems governed by non-Hermitian Hamiltonians. We argue that the Schwinger-Keldysh formalism gives a natural description for those problems. To be concrete, we study a simple model inspired by mesoscopic physics – an asymmetric junction (relevant to spin-valve devices). The system is governed by a non-Hermitian Hamiltonian which captures essential aspects of irreversibility. Calculated steady state transport properties show behavior which is anticipated on physical grounds.

12:51PM Q39.00009 ABSTRACT WITHDRAWN

1:03PM Q39.00010 Caliber approach for non-equilibrium systems with a small number of states, JEREMY SCHMIT, KINGSHUK GHOSH, KEN DILL, University of California, San Francisco — We present a theory for the dynamics of systems with a small number of states based on E.T. Jaynes' principle of Maximum Caliber. We construct the full dynamical partition function using a transfer matrix formalism with the transition rates as input parameters. Using this partition function, we are able to calculate all moments of dynamical quantities, and thus are able to predict fluctuations around the average behavior. We compare our results to single molecule and microfluidics experiments and contrast our results to the predictions of Minimum Entropy Production.

1:15PM Q39.00011 Transition rates for a Blume-Capel model coupled to a phonon bath, KYUNGWHA PARK, Virginia Tech — In nanoscale systems ranging from semiconductor quantum dots to arrays of magnetic nanoparticles or nanoscale magnetic molecules, dynamic properties play a crucial role in understanding the underlying physics and in designing systems of interest for applications. Dynamic properties are highly sensitive to transition rates used, so it is crucial to use a physically correct stochastic dynamic to examine dynamic properties. However, spin Hamiltonians do not provide generic dynamics, so a dynamic should be determined from microscopic Hamiltonians. As the first step towards deriving a realistic spin dynamic of nanoscale systems, we consider the ferromagnetic S=1 Blume-Capel model on a square lattice in which each spin is weakly coupled to a d-dimensional phonon bath, and derive transition rates from a spin-phonon coupling Hamiltonian. Based on the derived transition rates, dynamical properties such as metastability and nucleation are studied in the low-temperature limit using kinetic Monte Carlo simulations. The properties obtained from the phonon-assisted transition rates are compared with those from the Glauber transition rate.

1:27PM Q39.00012 Statistical mechanics far from equilibrium: prediction and test for a sheared system1, A. BAULE, R. M. L. EVANS, R. A. SIMHA, P. D. OLMSTED, University of Leeds — Beginning from a description of the forces of interaction between microscopic particles in motion, equilibrium statistical mechanics can predict both the statistical properties of their resulting configurations and the properties of the fluid (or other material) that they constitute. Despite the existence of statistical steady states of complex fluids under continuous shear flow, with intriguing similarities to equilibrium phase behaviour, a similar complete statistical solution has hitherto been unobtainable away from thermodynamic equilibrium. Instead, theorists have had to resort to artificial models with simple dynamics (e.g. some invented set of microscopic transition rates) or, alternatively, to use near-equilibrium approximations. We report the first complete statistical treatment of a collection of particles interacting via Newtonian forces in the presence of continuous boundary-driven flow, arbitrarily far from equilibrium [1]. Our investigation is based on a non-equilibrium counterpart to detailed balance [2] which leads to a set of simple constraints for the driven transition rates in our model system. We have tested the predictions in simulations, by numerically solving and time-stepping the force-balance equations. [1] R. M. L. Evans, R. A. Simha, A. Baule and P. D. Olmsted, to be submitted. [2] R. M. L. Evans, Phys. Rev. Lett. 92, 150601 (2004).

1:39PM Q39.00013 Dynamic phase transitions in model glass formers1, FRÉDÉRIC VAN WIJLAND, Laboratoire Matière et Systèmes Complexes, Université Denis Diderot - Paris VII — Glassy dynamics is identified through a series of signatures, such as aging, slow relaxation and the presence of dynamical heterogeneities. Basing our considerations on kinetically constrained glass formers, we argue that these phenomena are the byproduct of an intrinsically dynamic phase transition. The latter can be unravelled by performing, in the spirit of Ruelle, a Gibbs-like statistical mechanics over the set of time realizations of the systems’ evolution, rather than over the conventional set of phase space configurations.

1Work done in collaboration with J.P. Garrahan, R.L. Jack, V. Lecomte, E. Pitaud and K. van Duijneveldt

Wednesday, March 12, 2008 11:15AM - 2:03PM — Session Q40 DCMP: Metals: Nanoparticles, Compounds and Thermodynamics

11:15AM Q40.00001 Sintering Behavior of Metallic Nanoparticles1, MARTIN FENDRICH, RALF MEYER, RUSLAN ZINETULLIN, DIETRICH E. WOLF, PETER ENTEL, Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — Novel technological applications call increasingly for the controlled production of nanoparticles with well-defined physical properties. An important subject in this field is the sintering of agglomerated particles. We employ two different computer-simulation techniques to simulate the sintering of metallic nanoparticles. Molecular-dynamics simulations are used to study the early stage (t < 100 ns) of the sintering of two Ni nanoparticles with a size of about 4 nm. These simulations make it possible to observe important metallurgical details, like the role of (partial) dislocations in the process of the alignment of the crystal lattices. The data of the molecular-dynamics simulations are then used to calibrate the time-scale of kinetic Monte-Carlo simulations which can follow the sintering process over a much longer time-scale. A special technique is used in these simulations which makes it possible to take the misaligned crystal lattices into account.

1Supported by the Deutsche Forschungsgemeinschaft (SFB 445)
properties of PtSn

These results show that the EPI can influence the phonon thermodynamics at temperatures up to 1000 K. In their electronic DOS. The phonon-enhanced thermal smearing of these sharp features results in reduced screening of nuclear motions and stiffer phonons.

solid solutions, and for the A15 compounds V3Si, V3Ge and V3Co, at temperatures from 10 K to 1300 K. Pure V and the A15 superconductors V3Si and V3Ge

Inelastic neutron scattering was used to measure the phonon densities of states (DOS) for pure V and V-6%X

BRENT FULTZ, CALTECH, CALTECH TEAM — Inelastic neutron scattering was used to measure the phonon densities of states (DOS) for pure V and V-6%X

tured materials, CHRISTOPHER SALDANA, TEJAS MURTHY, Purdue University, RAVI SHANKAR, University of Pittsburgh, SRINIVASAN

At higher deformation rates under the same conditions, distribution of twin lamellae resulted in a thermally stable nanostructured material.

Amongst nano-grain boundaries through SPD at cryogenic temperatures. The stabilization in such a composite microstructure was traced to the peculiar

strength material systems. A novel stabilization route was discovered in these fine-grained systems when a high-density twin nano-lamella was introduced

CHANDRASEKAR, ERIC STACH, Purdue University — Intrinsic thermal instability of nanostructured metals have limited the applicability of these high-

Research Laboratory, TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — Nanoparticle

Nanocomposites, THOMAS EKIERT, GERALD POIRIER, KARL UNRUH, University of Delaware — Fe-Ag nanocomposites have been prepared by a transmutation reaction in which metallic Fe nanoparticles are used to reduce an aqueous solution of Ag+ ions. As the reaction proceeds, the Fe nanoparticles fragment into smaller particles and are reduced in size and metallic Ag nanoparticles are formed. The evolution in the structure and composition of the reaction products has been studied as a function of the time and the solution temperature by scanning and transmission electron microscopy, energy dispersive x-ray spectroscopy, and x-ray diffraction measurements. These measurements indicate that nearly all of the available Ag+ ions are reduced to metallic Ag within 5 minutes at solution temperatures between 5 °C and 35 °C. However, at higher solution temperatures the fragments of the Fe nanoparticles very quickly oxidize if the reaction is not carried out under anaerobic conditions. The magnetic properties of the Fe-Ag nanocomposites have also been studied by vibrating sample magnetometry. These measurements show a corresponding decrease in the saturation moment of those Fe-Ag nanocomposites not prepared under anaerobic conditions, with the majority of the change occurring within the first five minutes of exposure to the Ag+ solution.

Creation of low-energy twin lamellae for thermal stability in nanostructured materials, CHRISTOPHER SALDANA, TEJAS MURTHY, Purdue University, RAVI SHANKAR, University of Pittsburgh, SRINIVASAN CHANDRASEKAR, ERIC STACH, Purdue University — Intrinsic thermal instability of nanostructured metals have limited the applicability of these high-strength material systems. A novel stabilization route was discovered in these fine-grained systems when a high-density twin nano-lamella was introduced amongst nano-grain boundaries through SPD at cryogenic temperatures. The stabilization in such a composite microstructure was traced to the peculiar kinematic behavior of the twin-grain boundary triple junction. Copper was chosen as model material and deformed under cryogenic conditions using machining with varying deformation rates. The microstructure was investigated through HREM as a function of time and temperature. At small deformation rates, the SPD at cryogenic temperatures resulted in the creation of a nanostructured material with an unstable microstructure that coarsened even at room temperatures. At higher deformation rates under the same conditions, distribution of twin lamellae resulted in a thermally stable nanostructured material.

Electron-Phonon Interaction and High-Temperature Thermodynamics in Vanadium Alloys and Compounds, OLIVIER DELAIRE, MAX KRESCH, MATTHEW LUCAS, JORGE MUNOZ, CALTECH, JIAO LIN, BREN'T FULTZ, CALTECH, CALTECH TEAM — Inelastic neutron scattering was used to measure the phonon densities of states (DOS) for pure V and V-6%K solid solutions, and for the A15 compounds V3Si, V3Ge and V3Co, at temperatures from 10K to 1300K. Pure V and the A15 superconductors V3Si and V3Ge exhibit an anomalous anharmonic stiffening of phonons with increasing temperature up to 1000 K. In V, this anharmonicity is suppressed by Co and Pt, but not by iso-electronic Nb solutes. Non-superconducting V3Co exhibits a normal quasi-harmonic softening. The electronic density of states was calculated from first-principles DFT methods for all alloys and compounds. The materials whose phonons behave anomalously also exhibit sharp peaks below the Fermi energy in their electronic DOS. The phonon-enhanced thermal softening of these sharp features results in reduced screening of nuclear motions and stiffer phonons. These results show that the EPI can influence the phonon thermodynamics at temperatures up to 1000 K.

Remarkably large field dependences of the thermodynamic and transport properties of PtSn1, P.C. CANFIELD, S.L. BUD’KO, E.D. MUN, H. KO, G.D. SAMOLYUK2. Ames Lab / Iowa State University — PtSn1 is a known, binary, intermetallic compound that forms as a result of a deeply paritectic reaction. It’s reported to have an orthorhombic crystal structure with lattice parameters a = 6.42, b = 11.4, c = 6.39 Å. Exceptionally low residual resistivity single crystals of PtSn1 have been grown out of excess Sn (with RRR values larger than 1000) and a detailed study of their field dependent properties have been made. The highlights of our results can be summarized as follows: (a) PtSn1 manifests a huge, low temperature magneto-resistivity of 107 %, for an applied field of 5 T, that rises to 109 % for 14 T; (b) PtSn4 manifests dramatic and clearly resolved oscillations in the magnetization that, for fields below 7T, can be clearly resolved for temperatures as high as 20 K; (c) PtSn5 manifests dramatic and clear oscillations in electrical resistivity, that, for fields below 14 T, can be clearly resolved for temperatures as high as 10 K.

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

Scanning Tunneling Microscopy Atomic Resolution of Uranium Compound, MARILYN HAWLEY, SHAO-PING CHEN, Los Alamos National Laboratory, PHILLIP VAN STOCKUM, Stanford University — Room temperature ultra-high vacuum scanning tunneling microscopy (STM) atomic resolution imaging has been achieved for the first time on a layered uranium compound, uranium antimony two. High quality single crystals were cleaved in situ then imaged by STM using PtIr tips. Atomic resolution images revealed an in-plane square lattice with an uranium-uranium interatomic spacing consistent with theoretical predictions for the lowest energy cleavage plane. The STM images revealed a number of, as yet, unexplained features suggestive of missing atoms and single atom wide rows of atoms aligned along the two a-lattice parameter directions, which will be discussed in this talk.
1:03 PM Q40.00010 Structure of Boron Carbide: Where's the Carbon? , DAVID MARX1, Illinois State University, GERALD SEIDLER, TIMOTHY FISTER, KENNETH NAGLE, University of Washington, CARLO SEGRE, Illinois Institute of Technology — Although the structure of the boron carbide series, B\textsubscript{12}C\textsubscript{x}, with 0.06 < x < 1.7, has been studied since the 1940s, the location of the carbon atoms has not been adequately determined. The recent development of the lower energy resolution inelastic x-ray scattering (LERIX) spectrometer on the PNC-CAT beamline at the Advanced Photon Source at Argonne National Lab has enabled differentiation of the boron and carbon absorption edge data for the various crystallographic sites. The structure (R-3m) consists of twelve-atom icosahedra and three-atom chains. Boron carbide may have a maximum of three carbon atoms, which may be located on the two end of chain sites and in one of two inequivalent sites on the icosahedra. At least one carbon atom must be present in the structure for it to be stable. In this presentation, structural results from non-resonant x-ray scattering for seven samples, ranging from B\textsubscript{12}C to B\textsubscript{10}C\textsubscript{1}, will be presented.

1:15 PM Q40.00011 Electronic structure and properties of lanthanum . LANE NIXON, DIMITRIOSS PAPA-CONSTANTOPOULOS, George Mason University — The total energy and electronic structure of lanthanum have been calculated in the bcc, fcc, keps and dhcp structures for pressures up to 50 GPa. The full potential linearized augmented-plane-wave method was used with both the local-density and general-gradient approximations. The correct phase order has been found, with lattice parameters and bulk modules in good agreement with experimental data. The GGA method shows excellent agreement overall while the LDA results show larger discrepancies. The calculated strain energies for the fcc and bcc structures demonstrate the respective stable and unstable configurations at ambient conditions. The calculated superconductivity properties under pressure for the fcc structure are also found to agree well with experiments. Both LDA and GGA, with minor differences, reproduce well the experimental results for T\textsubscript{c}.

1:27PM Q40.00012 High-Level Correlated Approach to the Jellium Surface Energy, Without Uniform-Electron-Gas Input1 , LUCIAN CONSTANTIN, Tulane University, LUCIAN CONSTANTIN COLLABORATION, M. PITARKE COLLABORATION, J.F. DOBSON COLLABORATION, A. GARCIA-LEKUE COLLABORATION, J.P. PERDEW COLLABORATION — We describe the long-standing controversy over the surface energy of simple metals: Density functional methods that require uniform-electron-gas input agree with each other at many levels of sophistication, but not with high-level correlated calculations like Fermi Hypernetted Chain and Diffusion Monte Carlo (DMC) that predict the uniform-gas correlation energy. Here we apply a very high-level correlated approach, the inhomogeneous Singwi-Tosi-Land-Sjölander (ISTLS) method, and find that the density functionals are indeed reliable (because the surface energy is "bulk-like"). ISTLS values are close to recently-revised DMC values. Our work also vindicates the previously-disputed use of uniform-gas-based nonlocal kernels in time-dependent density functional theory.

1:39PM Q40.00013 Magnetic, thermodynamic and transport properties of GdFe\textsubscript{x}(Al\textsubscript{1-x}Zn\textsubscript{1-x})\textsubscript{2}0\textsubscript{1} . M. LAMPE, N. NI, N. JIA, G.D. SAMOLYUK, A.S. SEFAT, S.L. BUD’KO, P.C. CANFIELD, Ames Lab / Iowa State University — The unusual physical properties of the dilute, rare-earth-bearing, intermetallic compound GdFe\textsubscript{x}Zn\textsubscript{1-x}20\textsubscript{1} have been explained as being the result of the Gd\textsuperscript{3+} moment being embedded in a nearly ferromagnetic Fermi liquid. To understand this in detail, single crystals of the pseudo ternary series GdFe\textsubscript{x}(Al\textsubscript{1-x}Zn\textsubscript{1-x})\textsubscript{2}0\textsubscript{1} (x < 0.05) grown out of Zn-rich solution. Magnetization, heat capacity and resistivity measurements on these compounds reveal a decrease of T\textsubscript{c} from 86 K (x = 0) to 4 K (x = 0.07) for GdFe\textsubscript{x}(Al\textsubscript{1-x}Zn\textsubscript{1-x})\textsubscript{2}0\textsubscript{1} and a decrease of the Stoner enhancement factor, Z, from 0.88 (x = 0) to 0.35 (x = 0.05) for YFe\textsubscript{x}(Al\textsubscript{1-x}Zn\textsubscript{1-x})\textsubscript{2}0\textsubscript{1}. Rigid band approximation and TB-LMTO-ASA calculation are used to explain this trend. These results, combined with earlier studies of the substitution of Co for Fe clearly indicate the importance of band filling and the applicability of even a simple rigid band model, to these compounds.

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

1:51PM Q40.00014 Magnetic properties of RT\textsubscript{2}Al\textsubscript{20} (R = Gd, Eu and Yb, T = Ti, V and Cr) . J. FREDERICK, Ames Laboratory, USDOE, SHUANG JIA, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory, USDOE and Department of Physics and Astronomy, Iowa State University — Isotropical RT\textsubscript{2}Al\textsubscript{20} series of compounds contain less than 5 at. % of rare earth ions. Thermodynamic and transport measurements were performed on solution-grown, single crystals: both R = Gd and Eu series manifest clear local moment behavior with magnetic ordering below 10 K. These low transition temperatures are consistent with the dilute nature of the rare earth ions. Unlike the RT\textsubscript{2}Zn\textsubscript{20} series, we have not found enhanced magnetic order or near-Stoner like behavior for any member of the RT\textsubscript{2}Al\textsubscript{20} family of compounds. The R = Yb members, however, all manifest weak Pauli paramagnetism, consistent with a divalent state for the Yb ions.

1:00PM Session R1 APS: Poster Session III: 1:00 pm - 4:00 pm Morial Convention Center Exhibit Hall A

R1.00001 POLYMERIC AND ORGANIC MATERIALS II —

R1.00002 Ultrafast dephasing processes in β-carotene homologues , MASAZUMI FUJIWARA, KENSEI YAMAUCHI, MITSURU SUGISAKI, HIDEKI HASHIMOTO. CREST-JST and Department of Physics, Graduate School of Science, Osaka City University, RICHARD COGDELL, Institute of Biomedical & Life Sciences, Glasgow Biomedical Research Centre, University of Glasgow — Carotenoids is an important pigment in a bacterial light-harvesting system together with bacteriochlorophyll (BChl). In the photosynthetic system, these two kinds of pigments cooperate to efficiently capture the solar energy and to transfer energy to the reaction site within a few picoseconds. In this study, transient grating signals in β-carotene homologues using sub-20 fs excitation pulses were measured in order to investigate the dependence of the coherence dynamics on the conjugation length of these carotenoids. The conjugation length is a decisive factor in determining the efficiency of energy transfer to BChls. Therefore, it is important to study how the conjugation length affects the coherence dynamics. The results show that the population-induced dephasing is a major factor in the total dephasing process in the longer-chain carotenoids. On the other hand, pure dephasing time, which indicates the strength of the system-bath interactions, does not depend on the conjugation length. It is also concluded that the central C=C stretching mode is the major channel for energy dissipation to the environment regardless of the conjugation length.
R1.00003 Characterization of Bioderived Polyhydroxyalkanoates by Size Exclusion Chromatography, JOAN NEGULESCU, RAFAEL CUETO, KELLY RUSCH, TERESA GUTIERREZ-WING, BENJAMIN STEVENS, Louisiana State University Macromolecular Science Group — The plant derived polyesters, better known as polyhydroxyalkanoates, PHAs, are renewable and sustainable. \(-\text{O-CH}(-\text{CH}_2)_x-\text{CO-}N\). If \(x = 0\) PHA is Poly(lactic acid), PLA; if \(x = 1\) or \(2\) it is Poly(hydroxy butyrate), PHB, or Poly(hydroxy valerate), PHV. SEC and light scattering have been used before for determination of the absolute molecular mass of PLA dissolved in CHCl3 (Malmgren et al., J. Thermal Anal. Calorim., 2006, 83, 35-40). To our best knowledge there is no publication on the determination of the absolute MW of other PHAs. The bioderived polymers analyzed in this work were four catalog PHA samples: PHB Fluka 81329, PHB Natural Aldrich 363502, 95PHB/5PHV Aldrich 403105, and 92PHB/8PHV Aldrich 403113. SEC/LS instrumentation used: three Phenogel (1K-1000K) columns — a guard column, an Agilent pump and Wyatt Heleos MALS, QUELS (DLS), ViscoStar and rEX DRI detectors, all in series. The experimental dn/dc of PHB in CHCl3 (0.0936 ml/g at 658nm) allowed the determination of absolute MW of all PHA samples: PHB Fluka Mw 345,100 Mn 218,400; PHB Aldrich Mw 335,700 Mn 185,000; 92PHB/8PHV Mw 144,700 Mn 91,970; 95PHB/5PHV Mw 253,000 Mn 193,800.

R1.00004 Assembly of functionalized dicomponent nanorods at liquid-liquid and -air interfaces, BOKYUNG KIM, University of Massachusetts Amherst, SOOJIN PARK, DIAN CHEN, THOMAS MCCARTHY, THOMAS RUSSELL — Nanoporous templates are used to fabricate nanorods which have attracted significant interest for the fabrication of functional materials with interesting optical, electrical and magnetic properties due to their shape. We investigated a method for preparing well-ordered Anodized Aluminum Oxide (AAO) template using block copolymer micelles to transfer block copolymer patterns to the surface of aluminum as a mask during RIE. Electrochemical deposition was used to deposit Au blocks and poly(pyrrole) blocks into AAO templates to prepare dicomponent nanorods. Varying the diameter and length of them can be easily controlled by the hole diameter of AAO templates and the electropolymerization. By taking advantage of the different properties and functions of the individual components for offering additional degrees of freedom in self-assembly, their distinct surface chemistry was prepared. At liquid-liquid and -air interfaces, functionalized nanorods were distinctly self-assembled to adjust the interfacial strengths and stabilize two phases.

R1.00005 Fabrication of Highly Ordered Silicon Oxide Dots and Stripes from Block Copolymer Thin Films, BOKYUNG KIM, University of Massachusetts Amherst, SOOJIN PARK, JIAYU WANG, THOMAS RUSSELL — A general route to fabricate highly ordered arrays of nanoscopic inorganic oxide dots and stripes from block copolymer thin films is described. Poly(styrene-b-4-vinylpyridine) (PS-b-P4VP) thin films with cylindrical microdomains oriented normal and parallel to the surface were used as templates for the fabrication of nanoscopic silicon oxide. A thin PDMS layer was spin-coated onto the nanopatterned film, followed by thermal annealing. The PDMS diffused into the pores by capillary action. PDMS was transformed to silicon oxide by oxygen plasma treatment, while PS-b-P4VP was completely degraded, resulting in ordered arrays of silicon oxide.

R1.00006 Oscillatory jet flow in electrospinning of polymer nanofibers, SUREEPORN TRIPATANASUWAN, Department of Polymer Science, TheUniversity of Akron, DARRELL RENEKER, Department of Polymer Science, The University of Akron — The flow of polymer solution into an electrospinning jet can be controlled, the pressure applied to the fluid, and the flow out can be controlled by the electrical potential of the fluid. When the average flow rate of solution carried away by the jet was smaller than the rate at which the liquid was forced through the orifice into the jet, the solution flow rate and the electrical current both oscillated in time. The amount of fluid near the orifice grew larger and caused the flow out of that region to increase, and the amount of fluid near the orifice decreased. Then the cycle repeated. The oscillatory phenomena were demonstrated using a jet of polyethylene oxide in water (Molecular weight, 400k, concentration about 5%) flowing through a tube with a diameter of 0.7 mm. The pressure was 500 to 2500 Pascal, and the applied potential was around 5 kV. The frequency of oscillation (about 0.5 Hertz) was affected by the resistivity of the polymer solution (around 4500 ohm-meters).

1 We acknowledge financial support from the National Science Foundation, DMI-0600733.

R1.00007 Interaction Chromatography of Random Copolymers with Tunable Monomer Sequence Distributions, CHANG Y. RYU, JUNJONG HAN, BYUNG HO JEON, Rensselaer Polytechnic Institute, JAMES J. SEMLER, YOUNG K. JHON, JAN GENZER, North Carolina State University — We demonstrate that high performance liquid chromatography (HPLC) in the interaction chromatography (IC) mode is capable of distinguishing among various comonomer sequences in random copolymers (RCPs). A series of poly(styrene-co-4-bromostyrene) (PBrS), where \(x\) is the mole fraction of 4-BrS, RCPs have been prepared by brominating parent monodisperse polystyrene (PS). The distribution of S and 4-BrS segments in PBrS was adjusted by varying the molar ratio of S to PBrS before the bromination reaction. We utilize both normal and reversed phase IC techniques to demonstrate that the adsorption-based retention of PBrS RCPs is affected not only by their chemical composition, but also by the comonomer distribution in the RCP. Thus, IC can be used as a tool for material characterization. They provide information on the interplay between the macromolecular collapse and segment blockiness affected by the adsorption-based retention times in HPLC.

1 NSF PIRE and MOCIE (RTI04-01-04)

R1.00008 Polymorphism Control of Poly(vinylidene fluoride), JIANFEN ZHENG, AIHUA HE, JUNXING LI, CHARLES C. HAN, STATE KEY LAB OF POLYMER PHYSICS AND CHEMISTRY, INSTITUTE OF CHEMISTRY, CHINESE ACADEMY OF SCIENCES TEAM — Poly(vinylidene fluoride) (PVDF) is well-known for its polymorphism, and can exhibit five different polymorphs depending on its processing conditions. The \(\alpha\)-phase is the most common and stable polymorph and the \(\beta\)-phase is the most important one due to its piezoelectric and pyroelectric properties. Polymorphism control of PVDF has been realized through electrospinning. PVDF fibrous membranes with fiber diameter in the range of 100 nm to several micrometers were produced by electrospinning and the crystal phase of electrospun PVDF fibers can be adjusted at the same time. Through the control of electrospinning parameters such as the solvent and electrospinning temperature, PVDF fibrous membranes containing mainly \(\alpha\)-or \(\beta\)-or \(\gamma\)-phase could be fabricated successfully.

R1.00009 Role of Crystallinity in CNT Dispersion and Electrical Conductivity of SWCNT-Thermoplastic Nanocomposites, ADE KISMARAHARDJA, JAMES BROOKS, Florida State University, KEESU JEON, RUFINA ALAMO, FAMU-FSU College of Engineering — Using a homopolymer iPP and a series of propylene-ethylene random copolymers with a content of ethylene from 7 to 21 mol% as matrices, SWCNT nanocomposites have been prepared in a range of CNT concentration from 0.15 to 1 wt%. The poly(propylenes) have crystallinities ranging from 70 to 10 %, and serve to test the role of CNTs acting as nucleants to preserve the uniform dispersion of CNTs after sonication in solution. Growth of the semicrystalline structure from the nanotubes is a barrier to prevent CNT clustering. Less crystallizable polymers lead to composites with poorer dispersion and lower electrical conductivity. At SWCNT concentrations of 0.15wt%, SEM images of nanocomposites with the highest crystallinity matrix indicate de-bundled and uniformly dispersed nanotubes, while CNT aggregates remain in the lowest crystallinity nanocomposites. Electrical conductivity in the former is relatively high, while the latter are insulators. Also discussed is CNT dispersion from analysis of Raman spectra and polymorphism of the nanocomposites in relation to the unblended matrix.
Self-Assembling Semicrystalline Polymer into Highly Ordered, Microscopic Concentric Rings by Evaporation, MYUNGHWAN BYUN, SUCK WON HONG, Materials Science and Engineering Iowa State University, LEI ZHU, Materials and Biomolecular Engineering University of Connecticut, ZHIQUN LIN, Materials Science and Engineering Iowa State University, MYUNGHWAN BYUN, SUCK WON HONG, AND ZHIQUN LIN TEAM, LEI ZHU COLLABORATION — A drop of semicrystalline polymer, poly(ethylene oxide) (PEO) solution was placed in a restricted geometry consisting of a sphere on a flat substrate (i.e., sphere-on-flat geometry). Upon solvent evaporation from the sphere-on-flat geometry, microscopic concentric rings of PEO with appropriate high molecular weight were produced via controlled, repetitive pinning (“stick”) and denpinning (“slip”) cycles of the contact line. The evaporation-induced concentric rings of PEO exhibited a fibrillar-like surface morphology. Subsequent isotothermal crystallization of rings at 40 °C and 58 °C led to the formation of multilayer of flat-on lamellae (i.e., spiral morphology). In between adjacent spars, depletion zones were developed during crystallization, as revealed by AFM measurements. The present highly ordered, concentric PEO rings may serve as a platform to study cell adhesion and motility, neuron guidance, cell mechanotransduction, and other biological processes.

Drying-mediated Formation of “Coffee Rings” of Regioregular Conjugated Polymers, MYUNGHWAN BYUN, SUCK WON HONG, ZHIQUN LIN, Materials Science and Engineering Iowa State University, MYUNGHWAN BYUN, SUCK WON HONG, AND ZHIQUN LIN TEAM — A drop of semicrystalline conjugated polymer, regioregular poly(3-hexylthiophene) (rP3HT) toluene solution was allowed to evaporate from a confined geometry consisting of either a spherical lens or a cylindrical lens on a Si substrate (i.e., sphere-on-Si or cylinder-on-Si geometry). As toluene evaporated, mesoscale concentric “coffee rings” and fingers of rP3HT were formed as a result of controlled, repetitive “stick” and “slip” motions of the contact line. By tuning the interfacial interaction between rP3HT and the Si substrate, different surface morphologies were obtained as revealed by AFM measurements. The P3HT patterns formed on native silicon oxide surface exhibited nearly amorphous morphology, while nanorod-like structures were emerged on either HMDS treated or HF treated Si substrate.

New insight into surface melting in ultrathin polymer films: a combined surface x-ray scattering study, TADANORI KOGA, Chemical and Molecular Engineering Program, Dept of Mat. Sci. and Eng., Stony Brook University, Y. WANG, M. RAFAILOVICH, J. SOKOLOV, Dept of Mat. Sci. and Eng., Stony Brook University, A. TIKHONOVA, D. SCHULTZ, M. LEE, ChemMatCARS, The University of Chicago, X. LI, J. WANG, Advanced Photon Source, Argonne National Lab. — The crystallization of ultrathin polymer films on solid substrates has been studied for decades due to its importance in determining interfacial properties of coatings. Numerous groups have demonstrated that the rate of crystallization, crystal orientation, and density of nucleation points can be very different from bulk. We previously observed that, by using the shear modulation force microscopy (SMFM) measurements, the surface melting temperature \( T_s \) of polyethylene (PE) thin films decreased by 40 °C relative to the bulk melting temperature \( T_m \) when the thickness was close to the lamellar domain spacing (~15 nm). This large depression can’t be explained by the classical Thomson-Gibbs equation. In order to delve deeper into the mechanism of the surface melting, we integrated a variety of in-situ surface-sensitive scattering techniques, i.e., grazing-incidence x-ray diffraction (GID), grazing-incidence small-angle x-ray scattering (GISAXS), and diffuse scattering. We will present the detailed x-ray results and shed new light on the mechanism.

The Equilibrium Amorphous Fraction of Polymer Crystals, BUCKLEY CRIST, Northwestern University — Knowledge about disordered surfaces is important to the understanding of both melting and crystallization of polymer crystals. The concept of a surface roughening transition is well documented in atomic crystals; at sufficiently high temperatures, the entropic effects of a rough surface overcome the enthalpic penalty associated with atomic scale asperities. Similar effects operate when chain-like molecules crystallize. We concentrate fist on the basal surface perpendicular, or nearly perpendicular, to the molecular axes in extended chain crystals. In one case the positions of the chains are ideal, but liquid-like conformational defects are permitted near the surfaces. In the second case we add axial positional disorder to individual chains. Both models predict temperature-dependent equilibrium amorphous fractions (i.e., 0%, 1%, etc.) and could very different values. The study concludes with some comments about the equilibrium non-crystalline component of folded chain crystals.

Asymmetrical Functionalization of Nanoparticles Mediated by Polymer Single Crystals, BING LI, CHRISTOPHER LI, Drexel University — Considerable attention has been paid to nanoparticle (NP) research because of their fascinating properties and potential applications in nanotechnology and biotechnology. Asymmetrically functionalizing NP is of particular interest because it could directly lead to controlled patterning of NPs into complex structures for a variety of applications. Herein we report using 2-dimensional thiol-terminated poly(ethylene oxide) (HS-PEO) lamellar single crystals to immobilize gold NPs (AuNPs). Furthermore, this unique technique also enables asymmetric functionalization of AuNPs. Free-standing bilayer AuNP/PEO films were obtained. Dissolving PEO single crystals led to free asymmetrically functionalized AuNPs and AuNP complexes. The degree of functionalization (number of polymer chains per particle) can be readily controlled by tuning the molecular weight. The low molecular weight PEO undergoes integral folding, which leads to high areal density of thiol groups and thus the higher degree of functionalization, and vice versa. We anticipate that this methodology could be applied to other metal or semiconductor NPs.

Periodic Modification of Nanofibers by Polymer Crystallization, BINGBING WANG, CHRISTOPHER LI, Drexel University — Electrospinning polymer nanofibers are one of the most useful 1D nanometer-scaled materials that have numerous potential applications in the fields of filter applications, and templates for tissue engineering. Herein we show that polymer nanofibers can be used as 1D nucleation agents to induce polymer crystallization. Poly(ethylene oxide) was electrospun into nanofibers which was used to induce PEO crystallization in solution. Shish kebab morphology was observed with the nanofiber as the shish and the PEO lamellar crystals as the kebabs. This unique morphology was named as nano fiber kebab (NFSK). We demonstrated that the structural parameters of the NFSK such as the fiber diameter, periods, the kebab size etc. could be readily controlled by the electrospinning and crystallization conditions. This NFSK also renders 3D features to the otherwise 1D nanofibers. It also serves as a vehicle for incorporating a variety of functional groups to the nanofiber systems, which, in turn, leads to numerous biomedical as well as electronic applications.

Shear-induced orientation of poly(vinylidene fluoride-co-trifluoroethylene) thin films, HEEJOON JUNG, JIYOUN CHANG, CHEOLMIN PARK, yonsei university, NANOPOLYMERS LABORATORY, YONSEI UNIVERSITY TEAM — Control of molecular and micro structures of crystalline polymers, in particular in organic electronics, has been widely studied because of the significant influence of the electrical performance of polymers by the controlled structures. Shear technique has been known as one of the most effective methods for manipulating micro structure of many different polymers. The application of the shear method to polymer films is, however, very difficult of the thickness of less than 200nm. In order to utilize the shear method for polymer film, we designed a new shear apparatus. We have demonstrated global ordering of semi-crystalline P(VDF-TrFE), well known crystalline polymer for in non-volatile ferroelectric polymer memory, using simple static shear in large area of a few centimeter squares. The orientation, systematically examined as a function of shearing temperature, rate and film thickness, was elucidated by Atomic force Microscope and Field-Emission Scanning Electron Microscope and related to the ferroelectric polarization of a metal/ferroelectric/metal capacitor. In addition, the globally ordered thin film P(VDF-TrFE) crystal was characterized by Grazing Incident Wide Angle X-rays.
R1.00017 Surface Orientation in Injection-Molded Thermotropic Liquid Crystalline Copolyester (TLCP) Plaques. ROBERT BUBECK, Michigan Molecular Institute, JUN FANG, WESLEY BURGHARDT, Northwestern University, SUSAN BURGARD, KATHERINE ROBERTSON, Impact Analytical, DANIEL FISCHER, NIST — Attenuated total reflection Fourier transform infrared (ATR-FTIR) and 2D WAXS in transmission were used to characterize surface orientation in thermotropic liquid crystalline copolyester (TLCP) injection-molded plaques to varying depths into the samples. Injection-molded TLCPs have bimodal orientation states due to contributions from “skin” and “core” regions resulting from extensional and shear flow, respectively, in the mold. The NEXAFS is sensitive to the orientation of the molecular pi orbital of backbone phenyl groups of the top 2 nm of a surface. ATR-FTIR obtained using a Herrick SeagullTM variable angle reflectance accessory is sensitive for dichroic ratios to a depth of 5 microns. Orientation parameters derived from the 1502/cm absorption band for equivalent positions are often typically about 5 to 10 percent less by ATR-FTIR than by NEXAFS. The orientational states are being correlated with physical properties of injection-molded TLCP samples.

1 Research is supported by NSF grant #0521771.

R1.00018 Synthesis and Self-Assembly of Amphiphilic Protoporphyrin-Based Oligomers. JIAN-JUN MIAO, LEI ZHU, Institute of Material Science and Department of Chemical, Materials and Biomedical Engineering, University of Connecticut, STORRS, CT 06269-3136 — An amphiphilic discotic molecule based on asymmetric protoporphyrin has been synthesized by attaching two triethylene glycol monomethyl ether (TEG) chains to the two vinyl groups in protoporphyrin via bromination and etherification, followed by attaching two octadecylamine (ODA) chains to the two carboxylic acid groups in protoporphyrin via amidization. The purity of the sample was verified by 1H NMR, size-exclusion chromatography, and mass spectroscopy. Self-assembly in the solid state was studied by differential scanning calorimetry and X-ray diffraction (XRD). A broad melting peak was observed at ca. 100 degC, and a weak ordering was observed by XRD. Self-assembly in selective solvents was studied by dynamic light scattering and transmission electron microscopy. Large vesicles of 120 nm with a narrow distribution were observed.

1 This work was supported by NSF CAREER Award DMR-0348724.

R1.00019 Nanomechanical Measurements on Ultra-thin Poly(n-butyl methacrylate) Films. SHANHONG XU, GREGORY MCKENNA, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — The mechanical properties of ultra-thin poly (n-butyl methacrylate) (PBMA) films were investigated by the novel bubble inflation technique developed in our lab. Creep experiments were performed at temperatures above the glass transition temperature (Tg) of bulk PBMA. The deflection of the film is large enough to neglect the bending stiffness of the film. Surface effects were observed to play a much more important role in the inflation of the PBMA film, than had been observed for poly(vinyl acetate) (PVAc) and polystyrene (PS) previously investigated in our labs. Estimates of the surface energy contribution to film mechanical resistance for our measurements on PBMA are approximated 50% while those for PVAc and PS were between 8 and 31% depending on the details of the testing conditions including pressure and film thickness.

R1.00020 “Phase” Behavior of Aqueous Solutions of Poly(N-isopropylacrylamide). TOMOAKI KAWAGUCHI, Department of Polymer Chemistry, Kyoto University, Japan, KUNIHIKO KOBAYASHI, MASASHI OSA, TAKENAO YOSHIZAKI — A series of linear poly(N-isopropylacrylamide)(PNI Pam) samples were prepared by living anionic polymerization. The cloud-point curves for their aqueous solutions were determined by monitoring the transmittance of light through the solutions. The transmittance decreased monotonically with increasing temperature below the cloud point, as expected, but unexpectedly, it remained at a constant value if heating was stopped at a temperature. It means that the decrease in transmittance with increasing temperature does not necessarily correspond to the phase separation, i.e., the cloud-point curve for an aqueous solution of PNI Pam is not always identical with the coexistence curve.

1 This research was supported in part by the Global COE Program “International Center for Integrated Research and Advanced Education in Materials Science” from the Ministry of Education, Culture, Sports, and Technology, Japan.

R1.00021 Effect of Intermolecular Hydrogen Bonding on the Dynamics of Poly (2-vinylpyridine) Mixtures Containing Low Molecular Weight Phenolic Compounds. PORNPEN ATORNJAWAT, Burapha University, ROBERT KLEIN, Sandia National Laboratories, AMANDA MCDERMOTT, PAUL PAINTER, JAMES RUNT, Penn State University — The dynamics of poly(2-vinylpyridine) (P2VPy) mixed with a series of low molecular weight phenolic molecules (containing one to six hydroxyl groups) were investigated using broadband dielectric spectroscopy. All mixtures, FTIR spectroscopy indicates significant intermolecular H-bonding. All mixtures were single phase except for that containing 10 mol% hexahydroxybenzophenone, which formed a H-bonded complex with P2VPy. Intermolecular hydrogen bonding resulted in significant suppression of the P2VPy local relaxation in the glassy state. The segmental relaxations for mixtures containing 30 and 50% polyhydroxy compounds where broadened, indicating dynamic heterogeneity, whereas all P2VPy - ethylphenol mixtures exhibited dynamic homogeneity. Changes in relaxation strength of the segmental process are considered in light of calculated dipole moments for all species under investigation.

1 Supported by the NSF Polymers Program, DMR-0605027.

R1.00022 Small Angle Neutron Scattering of poly (ethylene oxide) ethyl alcohol / water mixtures. SANG HAK SHIN, ROBERT BRIBER, Materials Science and Engineering, University of Maryland, College Park, MD 20742, BOULEAM HAMMOUDA, DEREK HO, National Institute of Standards and Technology, Gaithersburg, MD 20899 — PEO solutions have interesting and complex features which arise from the interplay of the hydrophilic and hydrophobic sites on the chain (the oxygen atom and alkyl group respectively). PEO in ethanol forms an opaque gel-like mixture with a partial crystalline structure as confirmed by wide angle X-ray scattering. Addition of a small amount of water disrupts the gel: PEO in ethanol with 4 vol% water becomes a transparent solution. We confirmed the crystalline structure of PEO in ethanol and investigated the PEO chain conformation in mixed ethyl alcohol / water solutions using small angle neutron scattering (SANS). We also measured the phase behavior and spinodal temperature of PEO solutions in these mixed solvents with SANS. The phase behavior changes from an upper critical solution temperature (UCST) to a lower critical solution temperature (LCST) as the fraction of water is increased. The thermodynamic behavior changes from an UCST to LCST between 5~9% volume fraction water. PEO solutions which have more than 4~10 vol% water behave as an athermal polymer solution. The proposed origin of this unusual phase behavior comes from the formation of hydration layer around the PEO chain.
R1.00023 Multiscale Computer Simulation of Failure in Aerogels, BRIAN GOOD, NASA GRC — Aerogels have been of interest to the aerospace community primarily for their thermal properties, notably their low thermal conductivities. While such gels are typically fragile, recent advances in the application of conformal polymer layers to these gels has made them potentially useful as lightweight structural materials as well. We have performed computer simulations of aerogel thermal conductivity and tensile and compressive failure, with results that are in qualitative, and sometimes quantitative, agreement with experiment. However, recent experiments in our laboratory suggest that gels having similar densities may exhibit substantially different properties. In this work, we extend our original diffusion limited cluster aggregation (DLCA) model for gel structure to incorporate additional variation in DLCA simulation parameters, with the aim of producing DLCA clusters of similar densities that nevertheless have different fractal dimension and secondary particle coordination. We perform particle statics of gel failure on these clusters, and consider the effects of differing DLCA simulation conditions, and the resultant differences in fractal dimension and coordination, on gel strength and failure mode.

R1.00024 Active substrates through controlled creasing of surface-attached hydrogels, JUNGWOOK KIM, RYAN HAYWARD, University of Massachusetts, Amherst — A hydrogel film confined to a rigid substrate may undergo a mechanical instability to form sharp creases on its surface when placed under compressive stress. We will describe how this instability can be harnessed to generate substrates with surface chemical patterns that can be dynamically hidden and displayed. We employ lithographically micro-patterned underlying substrates as a route to spatially control the formation of creases. Using surface-bound hydrogels composed of poly(N-isopropylacrylamide), we prepare temperature-responsive dynamic substrates, whose surface reversibly fold and flatten as temperature is changed. Finally, deposition of polyelectrolytes on the hydrogel surface is exploited as a way to selectively pattern the surface chemistry of the gel. We focus on the use of poly(ethylene glycol) grafted polyelectrolytes with and without the integrin-binding peptide (RGD) as a route to dynamically control cell-substrate interactions.

R1.00025 Designing Surface Instabilities as Responsive Materials, EDWIN CHAN, JEFFREY KARP, ROBERT LANGER, Massachusetts Institute of Technology — Materials with surface properties that respond to external stimuli have potential applications as sensory devices, therapeutic materials and “smart” adhesive coatings. An example of a responsive material is a topographic surface whose pattern length-scale changes drastically in response to a stimulus. A potential approach to creating such a material is to take advantage of the morphological phase transition observed in elastic instability such as surface wrinkles. In this contribution, we present a general strategy to developing a responsive surface that takes advantage of this morphological transition in a poly(ethylene glycol) based elastomer. The responsiveness of this material is designed by the reversible transition between two distinct pattern length-scales; a small length-scale pattern of a microcels array that responds to an osmotic stress and leads to morphological phase transition to a large length-scale wrinkling pattern. Both these pattern length-scales are material’s defined since the microcels array forms naturally as a result of the residual stress that develops during polymerization, while the surface wrinkles forms due to the buckling stress that develops due to the applied osmotic pressure. Finally, we show that this phase transition occurs reversibly and demonstrate potential application of the material as an alternative design of a self-cleaning surface.

R1.00026 Correlation properties of dipole systems, YURI POPOV, PHILIP TAYLOR, Case Western Reserve University — We study theoretically the effects of electrostatic dipole-dipole interactions in ionomers, and the correlation properties of dipoles attached to either low-molecular-weight fluid or polymer chains. In particular, we study orientation-orientation correlations in systems of physical (extended) dipoles with relatively weak dipole moments. Correlation corrections to the free energy in such dipole systems are different from those in systems of point charges described by the Debye theory. The underlying physics, however, is similar: nearby dipoles rearrange around a given dipole in order to compensate for changes in its dipole moment and thus provide electrostatic screening. We develop both a simple Poisson-Boltzmann-like theory for such screening and a field-theoretic approach, which provides a natural language for describing such phenomena in a polymer context. New correlation lengths are obtained.

R1.00027 Micromechanics of Yielding for Ethylene / Methacrylic Acid Ionomers, ROBERT SCOGNA, RICHARD REGISTER, Princeton University — Partially neutralizing an ethylene/methacrylic acid copolymer (E/MAA) with either sodium or zinc leads to an increase in the yield stress, by an amount which increases with the level of neutralization. This is a direct consequence of increasing nanoscale heterogeneity: the formation of ion-poor and ion-rich domains within the amorphous phase of the ionomer. This segregation is evident by dynamic mechanical testing, which reveals that, upon neutralization, the $\beta$ relaxation peak of an unneutralized E/MAA copolymer splits into two parts which represent the relaxations in ion-poor and ion-rich regions. Though both sodium and zinc cations are capable of producing this segregation, the critical degree of neutralization required to produce the split relaxation is higher for zinc. The ion-poor relaxation occurs near the $T_g$ of low-density polyethylene while the temperature of the ion-rich relaxation increases monotonically with the degree of neutralization. Thus, increasingly higher temperatures or lower strain rates are needed to fully relax the ion-rich domains as the neutralization level is increased, resulting in the higher measured yield stress.

R1.00028 Ion Conduction and Polymer Dynamics of Poly(2-vinylpyridine) - Lithium Perchlorate Mixtures1, PORNKEN ATORNGITJAWAT, Burapha University, JAMES RUNT, Penn State University — Ion conduction and polymer dynamics of single phase mixes of poly(2-vinylpyridine) (P2VPy) with 0.1 to 10 mol% lithium perchlorate (LiClO$_4$) were investigated using broadband dielectric spectroscopy. Interpretation of the relaxation behavior was assisted by findings from wide-angle and small-angle X-ray scattering experiments, and other techniques. Five dielectric relaxations were observed: a local $\beta$ process in the glassy phase, a segmental relaxation, a slow segmental process, an ion-mode relaxation, and electrode polarization. The local P2VPy relaxation was strongly suppressed with increasing LiClO$_4$ content arising from the formation of transient crosslinks, which lead to a subsequent decrease in the number of free pyridine groups, and/or a reduction in the local free volume in the presence of LiClO$_4$. Ion conduction at low LiClO$_4$ concentrations (< 10 mol%) is governed by the diffusion of anions through the matrix, which is strongly coupled with the segmental relaxation. At relatively high LiClO$_4$ concentration (10 mol%), partial decoupling between ion motion and the segmental relaxation was observed, leading to increased conductivity.

1Supported in part by the NSF Polymers Program, DMR-0605627

R1.00029 Surface Structure of Ionic Liquids Determined by X-ray reflectivity and Sum-Frequency Generation Spectroscopy, DOSEOK KIM, YOONNAM JEON, JAEOH SUNG, Department of Physics and Program of Integrated Biotechnology, Sogang University, Seoul, Korea, WEI BU, DAVID VAKNIN, Ames laboratory and Department of Physics and Astronomy, Iowa State University, USA, YUKIO OUCHI, Department of Chemistry, Nagoya University, Japan — X-ray reflectivity and surface sum-frequency generation spectroscopy were used to study the surface of [BMIM][X] ionic liquids ([BMIM] = 1-butyl-3-methylimidazolium, X = BF$_4$, PF$_6$, and I). Sum-frequency signal strength from the terminal methyl groups of the cation at the surface indicates the topmost surface of these ionic liquids are occupied by polar-oriented hydrophobic butyl domains as the neutralization level is increased, resulting in the higher measured yield stress.
R1.00030 Surface Energy Effects on Polyelectrolyte Adsorption. RYAN J. MURPHY, VIVEK M. PRABHU, DENIS PRISTINSKI, ERIC K. LIN, N.I.S.T. - Polymers Division — Fluid-based directed assembly of functional nanoparticles is a promising approach to rapid fabrication of future devices. Current approaches of precise placement of these nanoscale building blocks onto pre-defined positions formed by lithography are of current interest. These methods allow for designer surfaces containing feature sizes both chemical and topological on the nanometer length scale. However, little is known about the kinetics of self assembly of charged macromolecular building blocks. Here, we investigate the adsorption kinetics of cationic polyelectrolytes as a function of surface energy, prepared by combinatorial methods. Ellipsometry and quartz crystal microbalance are used to understand the equilibrium and dynamic behavior. Constructing the adsorption phase diagram is a crucial first step towards developing a process mechanism for the directed assembly of nanoscale building blocks with polymers and nanoparticles as model systems.

R1.00031 Generating surface energy gradients for block copolymer thin film studies. JULIE LAWSON, THOMAS EPPS, Department of Chemical Engineering, University of Delaware — The development of block copolymer materials for future nanotechnologies requires an understanding of how surface energetics affect block copolymer thin film phase behavior. Surface energy gradients allow for combinatorial studies of these effects. In this work, surface energy gradients were created by vapor deposition of functionalized chlorosilanes on UVO-cleaned silicon substrates in a chamber under a dynamic vacuum process. The diffusion profiles of the chlorosilanes were controlled by the placement of the chlorosilane reservoirs in the chamber relative to the vacuum outlet and the substrate, allowing the profile of the surface energy gradient on the substrate to be tuned. X-ray photoelectron spectroscopy (XPS) was used to examine the results of the vapor deposition process. Additionally, thin films of a poly(styrene-b-methyl methacrylate) (PS-b-PMMA) block copolymer with a bulk cylindrical morphology were flow coated onto the gradient substrates, and the resulting phase behavior was characterized with atomic force microscopy (AFM).

R1.00032 Helix self-assembly through the coiling of cylindrical micelles. SHENG ZHONG, HONGGANG CUI, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware, ZHIYUN CHEN, KAREN WOOLEY, Center for Materials Innovation, Department of Chemistry and Department of Radiology, Washington University in Saint Louis, DARRIN POCHAN, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware — Both single and double helical superstructures with the length of several micrometers have been created through solution self-assembly of cylindrical micelles for the first time. Helical micelles which occur as a racemic mixture were formed from the co-assembly of poly(acrylic acid)-block-poly(methyl acrylate)-block-polystyrene triblock copolymers with triethylenetetramine or diethylenetriamine. Kinetic study reveals that the helix cylinders evolve from the stacking of intermediate micelle domains. The helix pitch could be efficiently adjusted by adjusting the amount and type of multiamine added. For example, the pitch distance would increase nearly 20% by increasing the relative molar amount of triethylenetetramine by 50% or substituting the tetraamine triethylenetetramine by the triamine diethylenetriamine. The helical structure exhibits unprecedented regularity for a nanostructure self-assembled from solution, which is proposed to be the result of long range electrostatic interactions coupled with uniaxial tension along the cylinder.

R1.00033 Self-assembled Patterns of Block Copolymer/Homopolymer Blends. DONG SIK PARK, EROL SANCÄKTAR, University of Akron, Poly. Eng. — The addition of homopolymer (Å) into an asymmetric triblock copolymer (ABA) increases the periodic orientation normal to substrate, enabling a directed self-assembly of the block copolymers into arrays of highly oriented, high-aspect ratio cylindrical nanostructure over large areas. The application of the physical properties of block copolymers provides substantial benefits in the nanotechnologies including nanostructured membranes, nanopatterns for nanoparticle synthesis, photonic crystals, and high-density information storage media.

R1.00034 UV-convergent One-loop Theory of Homogeneous Diblock Copolymer Melts. JIAN QIN, PIOTR GRZYWACZ, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — A renormalized one-loop theory is used to analyze collective and single chain correlations in the disordered phase of diblock copolymer melts. For chains with intermediate lengths (N ~ 1000), the deviation of the scattering intensity from predictions of the random phase approximation is found to be significant even far away from the mean field MST. The decrease in the wavenumber q* at which the scattering intensity is the maximum is shown to be a result of inter-molecular correlations, which leads to wavenumber dependent apparent q parameter, and to be unrelated to fluctuation-induced changes in single-chain correlations. The relationship to the Fredrickson-Helfand-Barrat theory is discussed.

R1.00035 Thin film effects on the morphology of diblock and triblock copolymers. KAREN SOHN, UCBS, KEN KOJIO, Nagasaki, ROBERT COFFIN, UCBS, BRIAN BERRY, NIST, GUILLERMO BAZAN, EDWARD KRAMER, UCBS, MICHAEL SPRUNG, JIN WANG, ANL — Surface effects in block copolymer thin films cause variations in the morphology from what is expressed in the bulk. The SEBS and SEB systems being studied have a composition such that both spherical and cylindrical morphologies are present in the bulk, depending on the annealing temperature. The bulk order-transition from cylinders to spheres occurs at 140°C, but in thin films the morphology is more dependent on film thickness and substrate characteristics than the annealing temperature. The morphology of thin films was studied on silicon oxide and polystyrene brushes using SFM and GISAXS. The polystyrene blocks of the SEBS and SEB were deuterated and then studied with d-SIMS in order to determine which block wets the interface with the substrate. For samples annealed at 180°C, SFM shows a cylindrical morphology on SiO2 substrates in the SEB, but a spherical morphology on the PS brush. GISAXS is used to determine whether the morphology is spheres or perpendicular cylinders. The SEBS shows a spherical morphology by SFM on both substrates.

R1.00036 A Comparative Study of Microphase Separation of Polyurethane Multiblock Copolymers with Different Soft Segment Chemistries. REBECA HERNANDEZ, CSIC Madrid, TAEYI CHOI, Penn State University, JADWIGA WEIKSLER, AJAY PADSALGIKAR, AorTech Biomaterials, LICHONG XU, CHRISTOPHER SIEDELECKI, JAMES RUNT, Penn State University — We focus in this study on three series of chemically well-defined polyurethanes (PUs) with the same hard segments (MDI-BDO) but different soft segment chemistries of interest in biomedical applications: 1000 g/mol aliphatic polycarbonate, polytetramethylenoxide and a mixed macrolol of polydimethylsiloxane (PDMS) and polyhexamethylenoxide. Using quantitative small-angle X-ray scattering we demonstrate that the degree of hard/soft segment demixing varies greatly between the materials. For example, the PDMS-based copolymers exhibit a three phase, core-shell morphology, while the other copolymers exhibit a typical two phase structure. Additional analysis was conducted with a number of experimental probes including FTIR to assess inter- and intracomponent hydrogen bonding, and tapping mode AFM to characterize the nanoscale morphology.

R1.00037 Hierarchical Self-Assembly of Block Copolymers for Lithography-Free Nanopatterning. SANG OUK KIM, BONG HOON KIM, Materials Science and Engineering, KAIST, South Korea, SANG CHUL JEON, National Nanofab Center (NNFC), Daejeon, South Korea — Development of a truly macroscopic scale nanopatterning process applying self-assembling materials has proved limited success. Hierarchical self-assembly is an alternative approach, which may produce complex architectures accommodating diverse functionalities. The mutually interacting multi-scale orderings of a hierarchical assembly may provide an opportunity to control over the diverse length scales simultaneously. We present lithography-free, truly macroscopic scale nanopatterning process utilizing hierarchical self-assembly of block copolymers. A micropatterned block copolymer film was self-organized from an evaporating block copolymer solution over an arbitrarily large area. The thickness modulation of the patterned film directed the spontaneous alignment of nanoscale morphology, producing a marvelous hierarchical morphology comprising microscale and nanoscale orderings. This facile and robust nanopatterning process employing the two levels of spontaneous orderings represents a versatile pathway to control nanoscale morphology by manipulating microscale architecture. Reference: B. H. Kim, et al. Adv. Mater. in press.

1 financial support: Samsung Advanced Institute of Technology (SAIT)
R1.00038 Block Copolymer Micelle Shuttles with Controllable Transfer Temperature between Ionic Liquids and Aqueous Solutions1. ZHIFENG BAI, YIYONG HE, TIMOTHY LODGE, University of Minnesota — Micelle shuttle is the term we used in our recent report that amphiphilic poly((1,2-butadiene)-block-ethylene oxide) (PB-PEO) block copolymer micelles (including spheres, cylinders, and vesicles) transfer, reversibly and with preservation of micelle structures, from an aqueous phase at room temperature to a hydrophobic ionic liquid at high temperature. We further found that the micelle shuttle could be realized in other ionic liquids, indicating its generality. The driving force for the transfer mainly originates from the deteriorating solvent quality of water for the PEO corona block at high temperature. The transfer temperature could be effectively tuned by adding ionic or non-ionic additives to the aqueous phase. Such an uncommon yet simple round-trip delivery system is of specific interest in quantitatively transporting solvophobic reagents, products, or byproducts between an ionic liquid reaction medium and an aqueous introduction or purification phase.

1This work was financially supported by the National Science Foundation through Award DMR-0406656.

R1.00039 Sphere-Forming and Cylinder-Forming Block Copolymer Thin Films Aligned Under Oscillatory Shear. ANDREW MARENCIC, RANULFO ALLEN, RICHARD REGISTER, Princeton University, PAUL CHAIKEN, New York University — Large-amplitude oscillatory shear has been shown to orient bulk block copolymers of spherical, cylindrical, or lamellar morphologies; however, no such experiments have been described for block copolymer thin films. Using oscillatory shear to orient microdomains would be advantageous in the creation of complex patterns especially in constrained geometries where simple shear is not possible. Here we demonstrate the ability to orient sphere-forming (trilayer) and cylinder-forming (monolayer) block copolymer thin films using oscillatory shear. The shearing field was applied to the thin film through a viscous fluid using a parallel-plate rheometer, allowing for continuous range of strain and shear rate. Real-space images were taken using atomic-force microscopy. As expected, a minimum strain within the film is required to induce ordering. We also observed that a larger stress is required to orient these thin films using oscillatory shear when compared to simple shear experiments. We also investigated how the ordering evolves with the number of cycles of shear applied to the film.

R1.00040 Hydrogenated ROMP Block Copolymers as Thermoplastic Elastomers. JOHN BISHOP, RICHARD REGISTER, Princeton University — Thermoplastic elastomers (TPEs) are typically symmetric ABA triblock copolymers made up of a “soft” rubbery midblock (B) and “hard” endblocks (A) that are usually glassy. We have used living ring-opening metathesis polymerization (ROMP) and subsequent hydrogenation to synthesize TPEs with semicrystalline “hard” blocks. The hydrogenated ROMP polymers we use include hydrogenated poly(methylacrylate) (hPMA), a highly crystalline polymer with \( T_m = 143 \)C; hydrogenated polyhexylmethacrylate (hPHM), a rubbery amorphous polymer with \( T_g = -22 \)C; and hydrogenated polyethylene glycol (hPEG), a glassy polymer with \( T_g = 183 \)C. The mechanical properties of our amorphous hPMMA-hPN-hPMMA TPEs, where microphase separation is driven by interblock repulsion, are comparable to commercially-available TPEs (also amorphous) at room temperature. In analogous hPMA-hPMMA-hPMA triblocks, where the endblocks are crystalline instead of glassy, microphase separation is driven by crystallization from a homogeneous melt, resulting in materials that are much easier to process, and with superior solvent resistance. However, the hPN endblocks show plastic deformation at moderate strains, yielding tensile strengths for the semicrystalline TPEs below those of their amorphous counterparts.

R1.00041 Composition Distributions and Effective Concentration of Miscible Polymer Blends Probed by MD Simulation. WENJUAN LIU, RALPH COLBY, Department of Materials Science and Engineering, The Pennsylvania State University, DMITRY BEDROV, Department of Materials Science and Engineering, University of Utah, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, THE PENNSYLVANIA STATE UNIVERSITY TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF UTAH TEAM — Using molecular dynamics we simulate the effects of thermally-driven concentration fluctuations and chain connectivity on segmental dynamics of miscible weakly interacting polymer blends. These naturally lead to local variations in glass transition temperature and hence, a distribution of segmental relaxation times. The self-convolution and pure component limits naturally truncate the Gaussian distribution of compositions surrounding a given segment. The most-probable composition differs considerably from the mean-field estimation of Lodge and McLeish for blend compositions that differ from 50/50, when we consider chain connectivity effects for all chains in the control volume.

R1.00042 Phase diagram of a binary liquid crystal mixture involving induced mesophase transitions1. TSANG-MIN HUANG, THEIN KYU, University of Akron, SHILA GARG, KATHY MCREARY, The College of Wooster, UNIVERSITY OF AKRON COLLABORATION, THE COLLEGE OF WOOSTER COLLABORATION — Phase transition temperature versus composition phase diagram of a binary nematic mixture (MBBA/5CB) has been established based on polarized optical microscopy and differential scanning calorimetry. The observed phase diagram is of an azeotrope type with a unique induced smectic phase, which is not present in neat constituents. This induced mesophase reveals a mosaic texture reminiscent of a smectic-B or a higher order smectic phase. At extreme compositions, the coexistence of nematic and solid crystal phases can be identified. Wide-angle x-ray diffraction was employed to determine the ordered mesophase structures. A theoretical model is being developed in the context of Flory-Huggins theory for liquid-liquid demixing in conjunction with a modified Maier-Saupe-McMillan theory to elucidate the interplay among nematics, higher order smectics, and eutectic crystals.

1Supported by NSF DMR 05-14942.

R1.00043 Dynamic Heterogeneity in Interacting Miscible Polymer Blends1. ASHISH GAIKWAD, TIMOTHY LODGE, University of Minnesota — Dynamic heterogeneity leading to time-temperature superposition (tTS) failure has been widely reported in non-interacting/weakly interacting miscible polymer blends. However, coupling of the component dynamic response in blends, even with a huge dynamic asymmetry in the pure components, is possible with H-bonding interactions. This study is focused on finding the minimum level of interaction necessary for thermo-rheological simplicity in blends. Blends of styrene-co-vinylphenol (PSVPh) and poly(vinyl methyl ether) (PVME) were chosen. Incorporation of styrene provides an effective way to modulate H-bonding interactions in the system. Linear viscoelastic data indicate that tTS fails for PS/PVME blends, whereas data obtained for different PVPh/PVME blends showed that tTS was obeyed over wide temperature range. For PVPh/PVME blends with low PSVPh content, tTS was successful. This suggests that the presence of alternating styrene and vinyl phenol units was insufficient for dynamic response decoupling. Further studies are in progress, with varying vinyl phenol content in PSVPh, to explore the influence of H-bonding on dynamic heterogeneity and blend dynamics.

1This work was financially supported by the National Science Foundation, through award DMR-0406656.
R1.00044 Induced Mesophase in Mixtures of Photopolymerizable Hyperbranched Polyester and Liquid Crystal Mesogen

NAMIL KIM, THEIN KYU, University of Akron, MAMI NOOAKA, HIROTO KUDO, TADATOMI NISHIKUBO, Kanagawa University — Phase behavior of a mixture of eutectic liquid crystals (E7) and hyperbranched polyester (HBPEAc-CoOH) has been investigated using polarized optical microscopy and differential scanning calorimetry. The observed phase diagram is an upper azeotrope, exhibiting the coexistence of nematic + isotropic phase in the vicinity of 90–110°C above the clearing temperature of neat E7 (60°C). With decreasing temperature a focal-conic fan shaped texture develops in the composition range of 70–90 wt% of E7, suggestive of induced smectic S_{α}. A phase in the mixture containing no known smectic phase in their neat forms. Wide angle x-ray diffraction (WAXD) technique revealed the existence of higher order mesophase(s). The phenomenon of induced mesophase in the hyperbranched polyester/E7 system will be discussed.

R1.00045 Interfacial slip in polymer blends with nanoparticles

JOSEPH ORTIZ, Dept of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794, EIHAB JABER, Dept. of Chemistry, Worcester State College, Worcester, MA 01602, DILIP GERSAPPE, Dept. of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794 — The interfacial region in polymer blends has been identified as a low viscosity region in which considerable slip can occur when the blend is subjected to shear forces. Here, we use Molecular Dynamics simulations to establish the role that added nanoparticles play in modifying the interfacial rheology. By choosing conditions under which the fillers are localized either in the two phases, or at the interface we can look at the interplay between the strengthening capability of nanoparticles, and the change in the interfacial slip behavior. We examine particle size, attraction between the particle and the polymer component and the amount of filler in the material. Our studies are performed both above and below the point at which the filler particles form a transient network in the blend.

R1.00046 X-ray characterization of hybrid PEO-clay nanocomposite films

EDUARD A. STEFANESCU, IOAN I. NEGULESCU, WILLIAM D. DALY, Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803 — The objective of the present contribution is to understand how clays with different chemistry, sizes and surface areas interact with each other and affect the structure and characteristics of polymer based nanocomposite multilayered films. In order to search for new synergistic properties and/or improve the properties of nanocomposite films already known, here we study polymer nanocomposites that have Laponite as well as Montmorillonite incorporated in various ratios. Although the polymer-clay solutions that are used to fabricate the nanocomposite films are completely exfoliated, XRD measurements confirm that all our dried multilayered films are highly exfoliated. Although the polymer-clay system per se has already been known, here we study polymer nanocomposites that have Laponite as well as Montmorillonite incorporated in various ratios. We use X-ray scattering to establish the role that the phase sequence of the multilayered samples plays in determining the mechanical properties of the multilayered films.

R1.00047 Interfacial and random field effects in polymers filled with nanoparticles

FOUAD ALIEV, VLADIMIR DOLIDZE, IVAN JOEL LOPEZ, University of Puerto Rico — We report on the influence of filling of poly(n-alkyl methacrylates) with nanoparticles on glass transition and relaxation processes, as investigated by dielectric spectroscopy and DSC. In order to estimate the role of interfacial effects at nanoparticle-polymer interface we used two types of Aerosil particles: with hydrophilic and hydrophobic surfaces. The agglomeration even of 2-3 volume percent of Aerosil particles in polymer forms a 3D-network dividing the polymer into random domains with liner size of several hundred nm, depending on the concentration of filling particles. The result of the filling of polymer is at least two fold: random field effects imposed by network and very developed area of the particles surface imposes interfacial effect on polymers. The relaxation times of α-relaxation process (sensitive to glass transition) in both filled polymers are faster than those of bulk polymers measured at the same temperatures. This might be interpreted as reduction of glass transition temperature in filled polymers. Semiquantitatively this reduction is in accordance with the Vogel-Fulcher data analysis of the temperature dependencies of bulk polymers measured at the same temperatures. Here, we extend these concepts to develop a model for the behavior of PNC T_{g}. The placement of impurities (nanoparticles) in a lattice (polymer matrix) changes the percolation threshold of the system, which we claim can be related to a change in T_{g}. Specific treatments of the impurities can result in either increases or decreases in T_{g} relative to the pure system, and the magnitude of the changes in T_{g} are related to the size and shape of the lattice impurities. We discuss the details of our results for such effects and compare them to experimental observations reported for PNCs.

R1.00048 Polymer nanocomposite (PNC) T_{g} from the perspective of percolation theory

JAMIE KROPKA, The University of Texas at Austin, PETER GREEN, The University of Michigan, VENKAT GANESAN, The University of Texas at Austin — A number of researchers have speculated on the connections between the liquid to glass transition and percolation concepts. Most recently, the film thickness dependence of T_{g} exhibited by polymers has been quantified in terms of the change in percolation threshold when transitioning from a 3D to 2D system. Here, we extend these concepts to develop a model for the behavior of PNC T_{g}. The placement of impurities (nanoparticles) in a lattice (polymer matrix) changes the percolation threshold of the system, which we claim can be related to a change in T_{g}. Specific treatments of the impurities can result in either increases or decreases in T_{g} relative to the pure system, and the magnitude of the changes in T_{g} are related to the size and shape of the lattice impurities. We discuss the details of our results for such effects and compare them to experimental observations reported for PNCs.

R1.00049 Effect of shear on the rheological and electrical properties of epoxy/MWCNTs dispersions

SAMEER S. RAHATEKAR, NIST, K. K. KOZIOL, ALAN H. WINdle, University of Cambridge, ERIK K. HOBie, Jeffery W. Gilman, NIST — We report the rheological, electrical and associated microstructural properties of multiwall carbon nanotubebased (MWCNTs) suspensions in an epoxy resin under shear. Above a critical concentration, we find a network of MWCNT aggregates with enhanced conductivity and viscosity. High shear results in MWCNT dispersion, with shear thinning and low electrical conductivity. The influence of MWCNT concentration and length on the scaling behavior of the elastic shear modulus is studied, and the role of individual MWCNTs is discussed. Further, we find significant differences in the scaling of the elastic shear modulus for different MWCNT lengths. Finally, we carry out small angle neutron scattering (SANS) in an attempt to establish a quantitative relationship between MWCNT microstructure and the corresponding rheological and electrical properties.

R1.00050 The amount of immobilized polymer in PMMA SiO\textsubscript{2} nanocomposites determined from caloricimetric data

CHRISTOPH SCHICK, ALBERT SARGSYAN, ANDREAS WURM, University of Rostock, Germany, SEVAN DAVTYAN, ANAHIT TONOYAN, SEUA, Yerevan, Armenia — The existence of an immobilized fraction in PMMA SiO\textsubscript{2} nanocomposites was shown on the basis of heat capacity measurements at the glass transition of the polymer. The results were verified by enthalpy relaxation experiments below the glass transition. The immobilized layer is about 2 nm thick at low filler content; agglomeration is not dominant. The thickness of the layer is similar to that found in semicrystalline polymers and independent of the shape of the nanoparticles. Nanocomposites therefore offer a unique opportunity to study the devitrification of the immobilized fraction (RAFT) without interference of melting of crystals as in semicrystalline polymers. It was found that no devitrification occurs before degradation of the polymer. No gradual increase of heat capacity or a broadening of the glass transition was found. The cooperatively rearranging regions (CCR) are either immobilized or mobile. No intermediate states are found. Sargsyan A, Tonoyan A, Davtyan S, Schick C. European Polymer Journal 2007-43:3113-3127.

R1.00051 ABSTRACT WITHDRAWN
R1.00052 “Cooperative” Relaxation Induced High Room-Temperature Dielectric
Constant in Supramolecular Diblock Copolymer Assembly

WEI CHEN, JIA-YU WANG, THOMAS RUSSELL, University of
Massachusetts, Amherst — The development of high-dielectric-constant polymers as active materials in high-performance devices is one of the challenges in
diﬀerent nanoscopic phases. Here, we report the development of high-dielectric-constant copolymers with a dielectric constant close to 50 at frequencies lower than 100 Hz. This is comparable with that of ferroelectric poly(vinylidene fluoride-
trifluoroethylene-chlorofluoroethylene) (PVDF-TrFE-CFE) terpolymer (40–60) and larger than those of PVDF (~10) and PVDF-TrFE (~20). Such a high
temperature-dielectric constant arises from the cooperative secondary relaxation between two blocks which increases the relaxation amplitude of CSA and
DY7, both of which have large dipole moments.

R1.00053 Electric Field Enhanced Diffusion of Salicylic Acid through Polyacrylamide Hydro-
gels
SUMONMAN NIAMLANG, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — The release mechanisms and the enhancement of salicylic acid - loaded polyacrylamide hydrogels were investigated experimentally by using a modified Franz-diﬀusion cell at 37 ◦ C to determine the eﬀects of crosslinking rate and electric field strength. A signiﬁcant amount of salicylic acid is released within 48 hours from the hydrogels of various crosslinking ratios, with and without electric ﬁeld. The release characteristic follows the Q vs. t^{1/2} linear relationship. Diﬀusion coeﬃcient initially increases with increasing electric
ﬁeld strength and reaches the maximum value at electric field strength of 0.1 V; beyond that, it decreases with electric ﬁeld strength and becomes saturated at electric field strength of 5 V. The diﬀusion coeﬃcient increases at low electric field strength (less 0.1 V) as a result of the electrophoresis of the salicylic acid, the expansion of pore size, and the induced pathway in pigskin. For electric field strength higher than 0.1 V, the decrease in the diﬀusion coeﬃcient is due to the pressure increase of the polyacrylamide pore size. The diﬀusion coeﬃcient obeys the scaling behavior D/D_0=(drug size/pore size)^m, with the scaling exponent m equal to 0.93 and 0.42 at electric ﬁelds of 0 and 0.1 V, respectively.

R1.00054 Induced Interaction of NH4NO3 With Poly(p-phenylene vinylene) by means of Ze-
olite Y. JIRARAT KAMONSANWAS, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — Conducting polymers are unique among the sensing materials known to us at present. They have many advantages over conventional metal sensors. Poly(p-phenylenevinylene) (PPV) can serve as the active material in sensor devices because PPV possesses good optical and electrical properties, and it can be synthesized by a relatively simple technique. Zeolite is chosen as inorganic ﬁller to be introduced into the conductive polymer matrix in order to increase electric sensitivity toward ammonium nitrate vapour. The objective of our work is to investigate the eﬀects of Si/Al ratio and cation type on the gas electrical conductivity sensitivity towards ammonium nitrate and corresponding interactions.

R1.00055 Styrene-Isoprene-Styrene Triblock Copolymer (SIS)/Polydiphenylamine Blends for
Actuator Application
KRAIPOP THONGSAK, ANUVAT SIRIVAT, The Petroleum and Petrochemical College — Styrene-Isoprene-Styrene triblock copolymer (SIS) is a dielectric material exhibiting many properties similar to polystyrene elastomer, which has been widely studied for electroactive applications. In our work, SIS films were prepared via ﬁlm casting at various polystyrene (PS) contents (19 wt. %, 29 wt. %, and 44 wt. %), yielding three diﬀerent morphology ﬁlms as characterized by an optical microscope, SEM, and TEM. Polydiphenylamine (PDPA), a conductive polymer, was synthesized by the oxidative polymerization and doped with HCl. For electroactive applications, electrochemical properties of pure SIS films and SIS/PDPA blends under stretching at a ﬁxed temperature of 25 ◦ C were measured to determine the eﬀects of morphology (spherical, cylindrical, and lamella morphology), particle concentration, and doping level on the electrochemical properties measured: the storage and the loss moduli (′G′ and ′G′), the storage modulus responses (∆G/2kV/mm), and the storage modulus sensitivities (∆G/2kV/mm/G/0), under applied electric ﬁeld strength varying from 0 to 2 kV/mm.

R1.00056 The eﬀects of monomer sequence distribution and isotopic substitution on solution
phase behavior of random copolymers
YOUNG KUK JHON, NCSU, RAMANAN KRISHNAMOORTI, U. of Houston, JAN GENZER, NCSU — We report on the eﬀect of chemical composition, co-monomer distribution and H/D isotopic substitution on the phase behavior in copolymers of poly(styrene-co-4-bromostyrene) (PBrS), where x denotes the mole fraction of 4-bromostyrene (4-BrS), in cyclohexane. By adjusting the solvent quality during bromination of parent polystyrene, either random or random blocky PBrS, (r-PBrS or b-PBrS, respectively), were synthesized. We studied the temperature dependence of phase behavior of PBrS with various x in cyclohexane as a function of the polymer concentration using light scattering. Our results reveal that for a given 4-BrS content, the cloud points of b-PBrS solutions are consistently higher and broader than those observed in r-PBrS solutions. The transition temperature has also been found to depend on the isotope substitutions of H or D in the polymer or the solvent. Small angle neutron scattering measurements indicate signiﬁcant diﬀerences in the temperature dependence of the thermodynamic behavior for the random and blocky samples and the nature of the ﬂuctuations upon approaching the phase boundaries.

R1.00057 The Antimicrobial Activity of Porphyrin Attached Polymers
LESLEY THOMPSON — We are interested in testing the antimicrobial activity of a porphyrin that is attached to a polymer. The porphyrin (5-(4-carboxyphenyl)-10,15,20-tris-(4-pyridyl)) was synthesized from methyl 4-formyl benzoate, 4-pyridinecarbonaldehyde, and pyrrole and attached to a copolymer of poly(styrene/poly(vinyl benzyl chloride), which was synthesized by free radical polymerization. The antimicrobial activity of the polymer-attached porphyrin was then determined for gram-negative E. Coli grown to 0.80 OD. In this procedure, glass slides were coated with polymer-attached porphyrin via dip-coating, and the E. Coli bacteria were plated in Luria Broth media. The plates were subsequently exposed to light overnight before they were incubated as porphyrins act as photo-sensitizers when irradiated with light. The polymer-attached porphyrin did exhibit antimicrobial activity and parameters that aﬀect its eﬃciency will be discussed.

R1.00058 Mesoscale Patterns Formed by Evaporation of a Polymer Solution in the Proximity
of a Sphere on a Smooth Substrate: Molecular Weight and Curvature Eﬀects
SUCK WON HONG, JIANFENG XIA, MYUNGHWAN BYUN, QINGZE ZOU, ZHIQUN LIN, Iowa State University — A drop of polymer solution was constrained in a sphere-on-flat geometry, resulting in a liquid capillary bridge. As solvent evaporated, intriguing surface patterns of polymer formed, which were strongly dependent on the molecular weight (MW) of polymer. Dotted arrays were formed at low MW; concentric rings were produced at intermediate MW; concentric rings, rings with fingers, and punch-hole-like structures, however, were yielded at high MW. Rings with fingers as well as punch-hole-like structures were manifestations of simultaneous occurrence of the “stick-slip” motion of the contact line and the fingering instabilities of rings. In addition, the curvature of the sphere in the sphere-on-flat geometry was found to aﬀect the pattern formation. A decrease in the curvature of the sphere led to an earlier onset of the formation of punch-hole-like structures when high-MW polymer was employed as the nonvolatile solute.
R1.00059 Thermal-reversible, size-selective desorption of nanoparticles from polymer brushes. RICHARD VAIA, STEVE DIAMANTI, Air Force Research Lab, WPAFB, SHAFI ARIFUZZAMAN, JAN GENZER, Dept. Chem. & Biomolec. Eng, NCsu — The ability to reversibly modulate surface energy and chemistry will provide new opportunities for future separation and sensing technologies. Post-polymerization functionalization of covalently-tethered polymer brushes affords a robust platform technology for these goals. Using standard succionimide-based coupling, hydroxyl pendants of poly(2-hydroxyethyl methacrylate) (PHEMA) brushes were conjugated to oligo-peptides, alkanes, fluoroalkanes, and oligo(ethylene glycol) (OEG) through an alpha-terthienyl primary amine. Coupling of these three different chemical moieties allows tailoring of the surface energy ($\gamma_{LV}^{\infty}$) $\sim$ 40-110 mJ/m$^2$, that combined with PHEMA grafting density and molecular weight (MW), leads to tunable adsorption of analytes. OEG-modified PHEMA brushes exhibit thermal-reversible desorption of analytes that is size-selective. For example, Au NPs of larger size are liberated from the brushes at shorter heating times; hence mixtures of Au NPs of different sizes can be sequentially released by controlling substrate heating. The impact of electrolyte content, Au NP surface chemistry, coupling efficiency and OEG MW is discussed to elucidate the detailed molecular mechanisms dominating the size and temperature-dependent OEG-Au NP binding efficiency.

R1.00060 SANS from CO$_2$-saturated coals at conditions relevant to subsurface sequestration. YURI MELNICHENKO, ORNL, ANDRZEJ RADLINSKI, Geoscience Australia, GANG CHENG, ORNL, MARIA MASTALERZ, Indiana Geological Survey, GEORGE WIGNALL, ORNL. — Carbon dioxide (CO$_2$) is the greenhouse gas which makes the largest contribution to global warming and roughly one third of the United States’ CO$_2$ emissions are generated by fuel-burning power plants. Capture and storage of CO$_2$ in underground geologic structures may significantly reduce CO$_2$ emissions to the atmosphere. Sequestration of CO$_2$ in mineable deep coal seams is particularly attractive as many coal-burning power plants are located near sites potentially suitable for geological storage. It is widely assumed that CO$_2$ can be captured and retained in coals by virtue of several mechanisms, such as fluid trapping of an “imobile phase” inside the pore space, adsorption to the pore surface and chemical bonding inside the organic coal matrix in the vicinity of pore walls. We report the results of the first small-angle neutron scattering (SANS) studies of several coals saturated with CO$_2$ at temperatures and pressures similar to those found in deep coal seams which are likely to be used for industrial-scale underground storage of CO$_2$. We found that the porous coal matrix may work to create absorbed fluid phase with the physical density much exceeding the density of the bulk fluid at the same thermodynamic conditions. Fluid densification is different in different coals which may explain the observed differences in sorption capacity and migration rates.

R1.00061 Selective excitation of excitonic transitions in PTCDA crystals and thin films. V.R. GANGILENKA, A. DESILVA, LYUBOV V. TITOVA, L.M. SMITH, H.P. WAGNER, Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221-0114, U.S.A., R. SCHOLZ, Walter Schottky Institute, Technical University of Munich, 80333 Munich, Germany. — We study various exciton transitions in PTCDA crystals and in thin films at low temperatures (≤ 5 K) by photoluminescence excitation spectroscopy (PLE) using DCM and RG6 dyes. The investigated PTCDA crystals are grown by sublimation and thin films are deposited on Si substrate by organic molecular beam deposition (OMBD) at high vacuum. The PLE excitation energy ranging from 1.878 to 2.172 eV enables the selective excitation of Frenkel excitons and of charge transfer transitions between PTCDA molecules in the same unit cell (CT1) as well as between stacked molecules along the growth direction (CT2). The observed excitation energy dependence of the emission bands supports the assignment of the different recombination channels obtained from time resolved PL measurements [1]. [1] A. Yu. Kobitski, R. Scholz, I Vragovic, H. P. Wagner, and D. R. T. Zahn, Phys. Rev. B 66, 153204 (2002).

R1.00062 Variable-Density Micelle Arrays in Block Copolymer Thin Films. JOHN PAPALIA, DOUGLAS ADAMSON, RICHARD REGISTER, Princeton University, PAUL CHAIRIN, New York University — Thin films of sphere-forming block copolymers are attractive templates for surface patterning and nanofabrication. Control over both the sphere (micelle) diameter and their average spacing (areal density). Within a given film, these quantities are statistically uniform: that is, there has not previously been a way to vary the number density of spheres across the film. By contrast, films having a thickness gradient are straightforward to prepare; however, regions of the film whose thickness is not commensurate with an integer number of layers of spheres will spontaneously form micron-scale islands or holes (terraces) of commensurate thickness, and a uniform areal density. By blending the block copolymer with matrix homopolymer, this terrace formation can be suppressed, so that creating a gradient in film thickness will also produce a gradient in micelle density. We employ a polystyrene-polysoprene diblock copolymer with block molecular weights of PS/PI 68/12 kg/mol, blended with PS homopolymer of varying molecular weights, in gradient films spanning thicknesses from 0-3 layers of spheres. At 50% PS homopolymer, terraces are still observed for homopolymer molecular weights in the “wet” brush region (9-50 kg/mol), but are completely suppressed when the homopolymer is excluded from the micelle corona (110 kg/mol).

R1.00063 ABSTRACT WITHDRAWN

R1.00064 Nanohole Structure in Polystyrene-block-poly(methyl methacrylate) Thin Film. WONCHUL JOO, SEUNG YUN YANG, JIN KON KIM, Pohang Univ. Sci. Tech., HIROSHI JINNAI, Kyoto Institute of Technology — Cylindrical nanoporous structures were prepared by using the mixture of polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) copolymer and PMMA homopolymer, and they were analyzed by using transmission electron microtomography and X-ray reflectivity. Two methods were employed for nanoporous structures: (1) whole PMMA phase was removed by UV irradiation and (2) only PMMA homopolymer was removed with selective solvent. We found that the nanoporous structure in the film prepared by method (1) exhibited cylindrical shape through the entire the film thickness. On the other hand, when the nanoporous film was prepared with the selective solvent, nanoporous structures exhibited a funnel-shape that the diameter of nanoholes located near the top of the film is larger than that located near the bottom of the film.

R1.00065 Thickness Dependence of Fluorescence Dynamics in Thin and Ultrathin Polystyrene Films. YOHEI TATEISHI, YOHEI OKADA, KEJII TANAKA, TOSHIHIKO NAGAMURA, Kyushu University — Fluorescence dynamics such as lifetime and rotational relaxation time for 6-(N-(7-nitrobenz-2-oxa-1,3-diazol-4-yl)amino) hexanoic acid (NBD) in polystyrene (PS) solid was examined as a function of film thickness, t. Both times decreased with decreasing thickness once the film became thinner than a critical value, t. Interestingly, in the case of ultrathin films, both times were insensitive to the film thickness. In addition, fluorescence intensity per unit thickness also decreased with decreasing thickness at t ≲ 50 nm, meaning that the fluorescence quantum yield was dependent on the thickness at t ≲ 50 nm. These results could be explained in terms of a simple three-layer model composed of surface, bulk and interfacial layers.

R1.00066 Interfacial Characterization of Poly(methyl methacrylate) with Non-solvents. YOSHI-HISA FUJII, HIRONORI ATARASHI, Kyushu University, MASAKIRO HINO, Kyoto University, KEJII TANAKA, TOSHIHIKO NAGAMURA, Kyushu University — Density profiles of a deuterated poly(methyl methacrylate) (dPMMA) film in water, hexane and methanol, which are “non-solvents” for dPMMA, were studied by neutron reflectivity (NR). The interfaces of dPMMA with the liquids were diffuse in comparison with the pristine interface with air; the interfacial width with water was thicker than that with hexane. Interestingly, in water, the dPMMA film was composed of a swollen layer and the interior region, which also contained water, in addition to the diffused layer. The interface of dPMMA with hexane was sharper than that with water. Although there were slight indications of a swollen layer for the dPMMA in hexane, the solvent molecules did not penetrate significantly into the film. On the other hand, in methanol, the whole region of the dPMMA film was strikingly swollen. The modulus of dPMMA in the vicinity of the interfaces with liquids was also examined on the basis of force-distance curves measured by atomic force microscopy. The modulus decreased closer to the outermost region of the film. The extent to which the modulus decreased in the interfacial region was consistent with the amount of liquid sorbed into the film.
R1.00067 Two photon absorption in PTCDA films using the z-scan technique, A.M. AWARD, V.R. GANGILENKA, Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, U.S.A., H. SCHMITZER, Department of Physics, Xavier University, Cincinnati, Ohio, 45207, U.S.A., H.P. WAGNER, Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, U.S.A. — The two-photon absorption coefficient of a polycrystalline PTCDA (pyrene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride) thin film was measured at 880 nm using the z-scan technique. The 2 µm thick PTCDA film was grown by organic molecular beam deposition (OMBD) on Pyrex. For the z-scan measurements ~1 ps pulses were focused onto the thin film using a microscope objective lens (100x) of numerical aperture 0.55 and a beam waist of 1 µm. The films have been moved by a translation stage with a travel range of 100 µm and with a step size of 0.5 µm. The two-photon absorption coefficient of PTCDA obtained from a fit with open aperture measurements at different intensities results to ∼100 cm GW⁻¹. The z-scan measurements demonstrate that crystalline PTCDA films possess strong nonlinear optical properties that might be utilized for optical applications.

R1.00068 Chemical Branching/Crosslinking of Preformed Polymers Using bis-Benzophenone1, NICHOLAS CARBONE, Columbia University, MARY DICKSON, Columbia University, JEFFREY COBERSTEIN, Columbia University — We show that bis-benzophenone (bis-BP) is an effective method to photochemically crosslink essentially any reformed polymer system that contains abstractable hydrogen atoms. When bis-BP is mixed into a polymer and exposed to UV radiation, it absorbs hydrogen atoms from any chains in proximity, thereby initiating a cascade of free radical reactions that include several mechanisms that can lead to covalent polymer crosslinking. Herein we study the early stages of branching reactions that precede gelation by following molecular weight changes in bis-BP modified polystyrene (PS) by Gel Permeation Chromatography. Quantitative molecular weight changes in PS-bis-BP thin films are studied as a function of irradiation time, PS-bis-BP molar ratio, and film height. AFM studies are employed qualitatively to investigate the relationship between molecular weight and the degree of dewetting of thin PS films deposited on silicon wafers.

1Research partially funded through NSF award IGER-0221589

R1.00069 Toward a minimum criteria of multi dimensional instanton formation for condensed matter systems?, ANDREW BECKWITH, APS/ Contractor, FNAL — We present near the end of this document a promising research direction as to how to generalize a technique initially applied to density wave current calculations to questions of instanton formation in multi dimensional condensed matter systems. Initially we review prior calculations done through a numerical simulation that the massive Schwinger model used to formulate solutions to CDW transport in itself is insufficient for transport of soliton-antisoliton (S-S’) pairs through a pinning gap model of CDW transport. Using the Peierls condensation methodology is implemented. The methodology is found to produce KWW fits of high accuracy. Moreover, the stretching parameter, β, is found to

R1.00070 The Anomalous Translocation Dynamics of Long-Chain Molecules, SRABANTI CHAUDHURY, BINNY J. CHERAYIL, Dept. of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India — Models of translocation based on simple Brownian diffusion mechanisms generally fail to account satisfactorily for anomalies in measured and simulated values of the average time of passage of long chain molecules through narrow pores. In an effort to rationalize these anomalies, we formulate an alternative model in which the time evolution of the number of monomers on one side of the pore is governed by the stochastic dynamics of a particle moving in a linear potential under the action of thermal fluctuations with long-ranged temporal correlations. We use this model in the limits of strong and weak diffusive bias to derive closed form expressions for the mean first passage time for pore crossing and the mean square displacement of a monomeric segment. These expressions, unlike those obtained from fractional Fokker-Planck formulations of the problem, are well-defined everywhere, and are also consistent with available numerical data.

R1.00071 Electric Field and Electron-Electron Interactions Effects on Bipolaron Transport in Polythiophene1, YAPING LI, JOLANTA LAGOWSKI, Memorial University of Newfoundland — Polythiophene is one of the most widely used organic conjugated polymer. Its charge transport mechanism has been a subject of many intensive studies. We employ the extended Su-Schriefer-Heeger’s theoretical model (SSH), including electric field and electron-electron interactions, to study bipolaron transport in polythiophene. This model involves the solution of coupled equations, consisting of the time-dependent Schrodinger equation and the classical motion equation for the lattice displacement, which are solved numerically in a self-consistent way. The time-dependent unrestricted Hartree–Fock approximation is also used. The parameters employed in the computations are determined by requiring good agreement with theoretical and experiment values for band gap and bond lengths. We find that a bipolaron does not distort significantly under weak electric field, however, a strong electric field can dissolve it, transforming localized charges into free charges. Electron-electron interactions do not significantly affect the nature of bipolaron transport in polythiophene.

1This work was supported in part by the National Science and Engineering Research Council of Canada.

R1.00072 Theoretical studies of the structures and optical properties of the dimers of the fluorene and carbazole derivatives, JOLANTA LAGOWSKI, Memorial University of Newfoundland, ZHIJUN GONG, Yangtze University — The intrinsic properties of the ground and excited states of fluorene, carbazole, fluorene-vinylene and fluorene-acetylene dimers and fluorene-carbazole unit are studied. The ground state optimized structures and energies are obtained using the molecular orbital theory and the density functional theory (DFT). The ground state potential energy curves of the dimers are also obtained. All molecules are nonplanar in their electronic ground states. The character and energy of the first 20 singlet-singlet electronic transitions are investigated by applying the time-dependent DFT approximations to the correspondingly optimized ground state potential energy curves of the dimers. The lowest singlet state is studied with the configuration interaction (singles) approach (CIS). CIS results suggest geometry relaxation in the first singlet excited state.

R1.00073 Orientational Relaxation in Simulated Polymer Melts, TAYLOR DOTSON, JOHN MCCOY, New Mexico Tech, JOANNE BUDZIEN, DOUGLAS ADOLF, Sandia National Laboratories, KEENAN DOTSON, JULIEANNE HEFFERNAN, New Mexico Tech — The orientational relaxation of simple polymer chains was studied using second Legendre polynomial autocorrelation functions. Such functions are commonly fit with a Kohlrausch-Williams-Watts (KWW) stretched exponential form. The value of the stretching parameter, β, and the degree that it changes as the glass transition is approached are both of physical interest. In the current project, a novel approach to determining the value and variation of β from molecular dynamics simulations is implemented. The methodology is found to produce KWW fits of high accuracy. Moreover, the stretching parameter, β, is found to collapse to a single-valued function of the decay timescale r regardless of thermodynamic path. Connections are drawn to experimental results and theoretical implications of the research are discussed.
align the orientation of block copolymer domain structures.

pattern. This result suggests that self-assembly of PS-PMMA can clean-up and interpolate the defects of patterned substrate while patterned substrate can

epitaxially-grown cylinder structures were well aligned with defect-free hexagonal lattice, although the chemically-patterned substrate have some defects in its

substrate and annealed to undergo microphase separation. The chemically patterned substrate was prepared by patterning polystyrene grafted silicon wafer

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mixed corona micelles with corresponding morphological changes, as evidenced in cryogenic transmission electron microscopy and dynamic light scattering.

u-EOF micelles with the cores consisting of E and F solvophobic cores, have received great interest recently. This novel type of micelle was first realized by the micellization of triptych triblock copolymers—u-EOF

MARC HILLMYER, TIMOTHY LODGE, Univ of Minnesota-Twin Cities — Multicompartment micelles, self-assembled nanoscopic aggregates with subdivided

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α

high-pressure vibrational spectroscopic studies of semi-crystalline polymeric materials such as revealed a crystalline phase transition in only one polymeric material, poly (tetrafluoroethylene), at high pressures. Since that time, however, there have been relatively few studies of high-pressure polymorphism in polymers, with the exception of experiments on polyethylene. Hence, there is still not a clear picture of how common structural phase transitions are at high pressure in polymeric materials, in contrast to the situation for small organic molecules. The results of

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microdomains were changed to hexagonally-packed cylinders. This is due to intra-chain coordination between CdCl

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electron microscopy (TEM). D-spacing of PS-P2VP coordinated with tiny amount of CdCl

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and pyridine ring.

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We thank AFRL for the support.

R1.00076 Brownian dynamics simulations of tethered polymers on curved surfaces , MARGARET LINAK, MARTIN KENWARD, KEVIN D. DORFMAN, Department of Chemical Engineering and Material Science, University of Minnesota — Surface tethered polymers are an important component in many physical systems, including coating applications, microfluidic devices, drug delivery vehicles and molecular targets in DNA microarrays. The recent renewed interest in low-density tethered polymers (i.e., below the characteristic surface density of a polymer brush) is partially attributed to their applicability in the latter circumstances. We present a study of an isolated polymer chain tethered to a curved, impermeable surface, where the radius of curvature is varied from highly convex, through flat, to highly concave. Utilizing Brownian dynamics simulations, we examine the equilibrium properties of the polymer as a function of its stiffness and molecular size, as well as, the degree (and sign) of the surface curvature. Our results for curved surfaces have potential implications in a number of microfluidic and biological systems.

R1.00077 Phase Behavior of Polystyrene-block-poly(2-vinylpyridine) coordinated by Metal Chloride1 , DONG HYUN LEE, WONCHUL JOO, JIN KON KIM, Pohang Univ. Sci. Tech., JUNE HUH, Seoul National University, DU YEOL RYU, Yonsei University — The morphology and order-to-disorder transition (ODT) of asymmetric polystyrene-block-poly(2-vinylpyr dine) copolymers (PS-P2VP) varying chain length of P2VP coordinated with CdCl

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were investigated by rheometry, synchrotron small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). D-spacing of PS-P2VP coordinated with tiny amount of CdCl

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increased greatly. With increasing amount of CdCl

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spherical microdomains were changed to hexagonally-packed cylinders. This is due to intra-chain coordination between CdCl

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and pyridine ring.

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This work was supported by Creative Research Initiative Program supported by KOSEF.

R1.00078 Vibrational Spectroscopy of Polymers at High Pressures1 , ERIK EMMONS, K.C. CHIARTKUNC-HAND, RICHARD KRAUS, JEFFREY THOMPSON, AARON COVINGTON, Physics Department and Nevada Terawatt Facility, University of Nevada, Reno — Vibrational spectroscopy of polymers at high pressures (>1 GPa) is an interesting but relatively unexplored field. Early studies by Bridgman in the 1940s revealed a crystalline phase transition in only one polymeric material, poly (tetrafluoroethylene), at high pressures. Since that time, however, there have been relatively few studies of high-pressure polymorphism in polymers, with the exception of experiments on polyethylene. Hence, there is still not a clear picture of how common structural phase transitions are at high pressure in polymeric materials, in contrast to the situation for small organic molecules. The results of high-pressure vibrational spectroscopic studies of semi-crystalline polymeric materials such as α- and β-poly (vinylidene fluoride) will be presented.

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Research supported by the U.S. DOE under grant DE-FG52-06NA27616 at UNR.

R1.00079 ABSTRACT WITHDRAWN —

R1.00080 Evolution of multicompartiment micelles to mixed corona micelles2 , CHUN LIU, ZHIBO LI, MARC HILLMYER, TIMOTHY LODGE, Univ of Minnesota-Twin Cities — Multicompartiment micelles, self-assembled nanoscopic aggregates with subdivided solvophobic cores, have received great interest recently. This novel type of micelle was first realized by the micellization of triptych triblock copolymers—u-EOF (E: polyethylethylene; O: polyethylene oxide; F: polyperfluoropropylene oxide) in aqueous solutions. u-EOF micelles with the cores consisting of E and F blocks underwent a gradual transition from nanostructured vesicles to segmented worms, and finally to multicompartiment “hammers” as the ratio of the hydrophilic O block to the hydrophobic E/F block increased. Herein, we report on the further manipulation of their structures via the introduction of a second solvent—tetrahydrofuran (THF), which is selective for both E and O blocks. As THF content increases, the micelles evolve from multicompartiment micelles to mixed corona micelles with corresponding morphological changes, as evidenced in cryogenic transmission electron microscopy and dynamic light scattering.

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This work was supported by the MRSEC program of the National Science Foundation under award DMR-0212302.

R1.00081 Control of microdomain orientations in block copolymer thin films with chemically-patterned substrate , MIKIHIITO TAKENAKA, SATOSHI AKASAKA, Kyoto University, YASUHIKO TADA, Hitachi Ltd., TOMOHIRO INOUE, Kyoto University, HIROSHI YOSHIUDA, Hitachi Ltd., HIROKAZU HASEGAWA, Kyoto University — We demonstrate defect-free and well-aligned self-assembly of cylindrical microdomains in block copolymer thin films on chemically-patterned substrates in arbitrarily large areas. Poly(styrene-b-methyl methacrylate) (PS-PMMA) with weight average molecular weight and weight fraction of PS being 6.7×103 and 0.69, respectively, was spin coated on chemically nano-patterned substrate and annealed to undergo microphase separation. The chemically patterned substrate was prepared by patterning polystyrene grafted silicon wafer by conventional electron beam lithography, to form hexagonally arranged circular areas having higher affinity to cylindrical microdomain forming blocks. The epitaxially-grown cylinder structures were well aligned with defect-free hexagonal lattice, although the chemically-patterned substrate have some defects in its pattern. This result suggests that self-assembly of PS-PMMA can clean-up and interpolate the defects of patterned substrate while patterned substrate can align the orientation of block copolymer domain structures.
R1.00087 Control of the processing window for block copolymer nanostructures by the addition of a homopolymer. JUNHAN CHO, Dankook University, DU YEOL RYU, Yonsei University, KWANG HYUN SONG, SANG BO NA, Dankook University, YOUNGMIN KIM, Hongik University — Processing window for block copolymer nanostructures is often limited by a material at hand and effective intermonomer interactions. Taking polystyrene-b-poly(methyl acrylate) (PS-b-PMMA) as a model system, it is one of the most widely used passive electronic materials, we investigated how to control the processing window for fabricating nanostructures from PS-b-PMMA by the addition of PS homopolymer. The ordering transition points were measured for the neat copolymer and its mixtures by optical and radiation scattering methods. A molecular model based on a random-phase approximation theory was then used to elicit the effective interactions between constituent blocks and to predict the measured ordering transition temperatures for the design and fabrication of nanostructures from the copolymer system at desired processing condition.

R1.00083 Order-to-disorder Transition on PS-b-PI Copolymer Thin Film. CHANGHAK SHIN, HYUNGU AHN, DU YEOL RYU, Yonsei University, KWANG-WOO KIM, Pohang Accelerator Laboratory, YONSEI UNIVERSITY COLLABORATION, POHANG ACCELERATOR LABORATORY COLLABORATION — The phase separation transition in thin film system has been studied for diblock copolymers poly(styrene-isoprene) [PS-PI]. It has been broadly known that the microphase-separated or ordered state for block copolymers possesses a lower average density than the disordered state due to the dominant entropic contribution to the free energy. In this study, we used ellipsometry to probe transition temperatures in block copolymer thin films because it makes use of the change in polarization induced upon the reflection light from a covered substrate and allows the calculation of the thickness of the film. The phase behavior is compared based on the volumetric change on transition.

R1.00084 Surface Neutrality for PS-b-PMMA Copolymer Thin Film. SUJIN HAM, EUNHYE KIM, CHANGHAK SHIN, DU YEOL RYU, Yonsei University, CRAIG HAWKER, University of California, Santa Barbara, CA, THOMAS RUSSELL, University of Massachusetts, Amherst, MA, YONSEI UNIVERSITY COLLABORATION, UNIVERSITY OF CALIFORNIA, SANTA BARBARA COLLABORATION, UNIVERSITY OF MASSACHUSETTS, AMHERST COLLABORATION — Many attempts were made to control over the microdomain orientations of block copolymers in the thin films such as application of strong electric field, solvent annealing and chemical modification of the substrate surface because a variety of nanoscale periodic patterns of the block copolymers offers the potential use as nanolithographic templates, data storage, electronics and membranes. From this study, we suggest the experimental surface conditions for neutrality based on PS/PMMA. Lamellar or cylinder-forming PS-b-PMMA copolymers were used to investigate the thickness dependence of the perpendicular orientation of the microdomains by varying the chemical compositions (PS/PMMA) of underlying random copolymer brushes. The brush surfaces modified by the random copolymers were obtained by thermal annealing due to simple chemical reaction. From the thickness windows for the perpendicular orientation in PS-b-PMMA thin films, the real neutral surface could be observed.

R1.00085 Optical Absorption and Emission of Fully Conjugated Heterocyclic Aromatic Rigid-rod Polymers Containing Sulfonated Pendant Groups. SHIH JUNG BAI, SHEN-RONG HAN, INSTITUTE OF MATERIAL SCIENCE AND ENGINEERING, National Sun Yat-sen University — Fully conjugated poly(1,7-dihydrobenzo[1,2-d:4,5-d’]imidazole-2,6-diyi)-2-(2-sulfophenylene) (sPBI) has a para-catenated rod-like backbone, which was synthesized and fabricated for mono-layer polymer light-emitting diode (PLED) showing a threshold voltage of 4.5 V and a green light (530 nm) emission. Its SO₃H moieties attached to the p-phenyl ring improved electron delocalization along the backbone resulted in a red shift of absorption spectrum. sPBI was further derivatized for rigid-rod polyelectrolyte sPBI-PS(Li⁺) by attaching propanesulfonated pendant to the heterocyclic moiety of intractable sPBI for water solubility. This fully conjugated polyelectrolyte sPBI-PS(Li⁺) was fabricated for light-emitting electrochemical cells (PLECs) with a dopant of LiCF₃SO₃ or Li[N(CF₃SO₂)₂] for effects of propanesulfonated pendant and lithium dopants on luminescent emission and on room-temperature conductivity. sPBI-PS(Li⁺) PLECs doped with 0.41 and 1.01 wt.% of Li[N(CF₃SO₂)₂] showed higher green light (514 nm) electroluminescence emission intensity with a threshold voltage of 3.0 V and -4.6 V, respectively. Emission intensity of the sPBI-PS(Li⁺) PLEC did not raise upon increasing the conductivity of the luminescent layer.

R1.00086 Non-linear V-I Characters of LSMO/PAn/Co/Al Organic Spin-Valve. Z.L. LIU, H.G. CHENG, Z.H. QIN, J. CHEN, X.J. WANG, Huazhong University of Science and Technology — The present paper used the magnetron sputtering and Sol-Gel method to prepare the organic-spin valves composed of La₀.₇Sr₃₋ₓMnO₃ (LSMO)/polyaniline (PAN)/Co/Al. We adopted the four probe to study the MR of the spin valve and observed the non-linear V-I characters. The TMR effect in the organic spin valve was also studied.

R1.00087 Electroluminescence of Conjugated Rigid-rod Polymer Tuned by Emission Layer Thickness. SHIH JUNG BAI, HUA-WEI TSENG, Institute of Materials Science and Engineering, National Sun Yat-sen University, JEN-WEI HUANG, Department of Chemistry, ROC Military Academy — Bilayered light emitting diodes were fabricated with fully conjugated rigid-rod polymer poly-(p-phenylenebenzobisoxazole) (PBO) on top of hole conducting poly(3,4-ethylene-dioxythiophene:poly(styrene sulfonate) (PEDOT-PSS) using indium-tin-oxide on glass as the substrate and also the electron injecting cathode. The hole injecting anode was Al vacuum evaporated onto the PEDOT-PSS layer. Electroluminescence emission was obtained showing a blue shift in emission wavelength greater than a threshold voltage for the bayered polymer diodes having a smaller PBO layer thickness. When the PBO thickness changing from 90 nm to 27 nm with a constant PEDOT-PSS layer thickness of 54 nm, the ΔVthreshold were 70 nm and 3.5 V, respectively.

R1.00088 Growth Kinetics of Au Nanoparticles: Mean Field Modeling and SAXS. HILMAR KOERNER, AFRL, MICHAEL TAMBASCO, Columbia University, ROBERT MACCUSPIE, RICHARD VAIA, AFRL, SANAT KUMAR, Columbia University, AFRL, WPAPB, OH TEAM, COLUMBIA UNIVERSITY, NY TEAM — Gold (Au) nanoparticles (NPs) are a mainstay of current nanoscience and technology. With such a diversity of applications, developing a better understanding of the impact of macromolecular additives on single-phase fabrication routes, and ultimately on the resultant interfacial composition and structure (size, shape and dispersity), is critical to optimize performance and lower production cost. In-situ small-angle x-ray scattering (SAXS) is uniquely situated to directly monitor the morphological evolution of Au NPs from single phase reduction of Au(I) by tert-butylamineborane. Deconvolution of the in-situ SAXS profiles provides direct information on the evolution of NP size, polydispersity and relative number density, as well as the on-set of clustering and superstructure formation. The size-time profiles agree with mean-field calculations elucidating the role of ligands, their length and structure on the nucleation and growth kinetics as well as thermodynamic and structural characteristics of the Au NPs. In general, the combined approach provides new insights on the impact of additives on the various stages of NP formation and the ability to quantify particle-pair potentials and ascertain impact on assembly – de-assembly process of NP superstructures.
R1.00089 Effect of Ligand Molecular Weight and Nanoparticle Core Size on Polymer-Coated Gold Nanoparticle Location in Block Copolymers. JOSHUA PETRIE, UC Santa Barbara, BUMJOON KIM, UC Berkeley, GLENN FREDRIKSON, ED KRAMER, UC Santa Barbara — Gold nanoparticles modified by short chain polymer thioles [Au-PS] can be designed to strongly localize in either domain of a polystyrene-b-poly(2-vinylpyridine) [PS-PVP] block copolymer or at the interface. The P2VP block has a stronger attractive interaction with bare gold than the PS block. Thus, when the areal chain density $\Sigma$ of end-attached PS chains falls below a critical areal chain density $\Sigma_c$ the Au-PS nanoparticles adsorb to the PS-b-P2VP interface. The effect of the polymer ligand molecular weight on the $\Sigma_c$ has been shown to scale as $\Sigma_c \sim (R_g/R_{\Sigma_p})^2$, where $R$ is the curvature of the Au nanoparticle core radius. To test this scaling relation for $\Sigma_c$ further we are synthesizing gold nanoparticles with different core radii and will present preliminary results on $\Sigma_c$ as a function of $R$.

R1.00090 Patternning of Nano-Objects on PS-b-PMMA Thin Films by Selective Swelling. KOOKHEON CHAR, JEONG GON SON, Seoul National University, PAUL F. NEALEY, HUIMAN KANG, University of Wisconsin — Nano-objects have recently received great attention due to their unique photonic, electronic, and magnetic properties. However, in order to take full advantage of these properties of nano-objects, massively parallel assembly or integration of nano-objects is required. Block copolymers are well known to spontaneously form a wide range of nanostructures and block copolymer thin films can easily allow nano-scale patterns. In this presentation, we would like to introduce a new approach to realize nano-object patterning on perpendicularly oriented polystyrene-block-poly(methyl methacrylate) thin films. Our main idea is based on the properties of block copolymer thin films that simultaneously form the topographical and chemical patterns. We employed the annealing with selective solvents to realize topographical patterns of block copolymer thin films, from which we realized nano-object patterns either in the grooves of the patterns or on the top of the patterns. We verified the structures and mechanisms for the nano-object patterns on block copolymer thin films using Atomic Force Microscopy, Field-Emission Scanning Electron Microscopy and X-ray Photoelectron Spectroscopy.

R1.00091 Target site search strategy of gene regulatory proteins. ANDREW SPAKOWITZ, MARIO DIAZ DE LA ROSA, Stanford University — Gene expression is orchestrated by a host of regulatory proteins that coordinate the transcription of DNA to RNA. Regulatory proteins function by locating specific binding sequences of DNA and binding to these sequences to form the transcription initiation complex. In many instances, these regulatory proteins only have several specific copies that must efficiently locate target sequences on the genome-length DNA strand. The non-specific binding of regulatory proteins to random sequences of DNA is believed to permit the protein to slide along the DNA in a stochastic manner. Periodically, a thermal kick or an interaction with another bound protein will disengage the regulatory protein from the DNA surface, leading to three-dimensional diffusion. Eventually, the protein will reattach to the DNA at a new location that is dictated by both the diffusivity of the protein and the DNA configuration. Cycling through these random events constitutes a search strategy for the target site. We build a reaction-diffusion theory of this search process in order to predict the optimal strategy for target site localization. The statistical behavior of the DNA strand acts as a necessary input into the theory, and we consider several governing behaviors for the DNA strand. We explore the impact of DNA configuration on target site localization in order to predict how protein expression will vary under different experimental conditions.

R1.00092 Conformational Dynamics and Interactions of a DNA Aptamer Observed by Single Molecule Spectroscopy. JAMES TAYLOR, QOSAI DARUGAR, AJISH POTTY, RICHARD WILLSON, CHRISTY LANDES — Single molecule fluorescence resonance energy transfer (FRET) and fluorescence correlation spectroscopy (FCS) are used to study the interactions and structural dynamics of a DNA aptamer. Studies are performed in the presence of and in the absence of the aptamer’s binding target, the dimeric form of vascular endothelial growth factor (VEGF) protein. FRET and FCS experiments are conducted to determine the characteristics of conformational fluctuations by the “aptamer-VEGF” complex under different two- and three-dimensional conditions. It is shown that the VEGF has conformational fluctuations on a relatively fast time scale (single milliseconds to tens of milliseconds), and that these fluctuations are largely counterion dependent, being especially sensitive to Mg$^{2+}$ concentration. While these fluctuations also occur in the presence of VEGF, results show that the dynamics occur on a slower time scale (hundreds of milliseconds to seconds), indicating that there is indeed an interaction between the aV aptamer and its binding target, VEGF.

R1.00093 Scaling Exponents for Polymer Translocation through a Nanopore. KAIFU LUO, TAPIO ALA-NISSILA, Helsinki University of Technology, PAWEL POMORSKI, MIKKO KARTTUNEN, University of Western Ontario, SEE-CHEN YING, Brown University, ANIKET BHATTACHARYA, University of Central Florida – We present results of extensive computer simulations and scaling theory for computing the relevant scaling exponents associated with polymer translocation through a nanopore [1]. We present results for the scaling of the average translocation time and the fluctuation in the reaction coefficient for the case of spontaneous and field-driven translocation in 2D and 3D. The models used include: (i) the fluctuating bond model with single-segment Monte Carlo moves, (ii) Langevin dynamics, and (iii) GROMACS MD simulations using the bead-spring model for flexible polymers without an explicit solvent. We contrast our results to the recently presented alternate theories for polymer translocation [2,3].


R1.00094 Stretch-Induced Density fluctuations in glassy polymers. MIKIHITO TAKEKANA, SHOTARO NISHIT-SUJI, SHIMIZU HIRONOFUMI, Kansai University, SHIHYA YOSHIOKIO, Osaka City University — Glassy materials are hard but fragile. The fragileness of glass strongly depends on its processing and the heterogeneity developed during the processing in glass materials may be important in its destruction under deformation. However, the mechanism how the heterogeneity develops and leads to the fragmentation or cracking is not well understood. Here we show that the stretch induced the violent of the incompressibility by the coupling between the stretch and density fluctuations due to the strong density dependence of viscosity in glassy polymer. We demonstrate that the small-angle X-ray scattering intensity of a glassy polymer increases with stretch and exhibits so-called butterfly pattern. This butterfly pattern arises from the competition between the stretch and density fluctuations under different two- and three-dimensional conditions. It is shown that the VEGF in the absence of VEGF has conformational fluctuations on a relatively fast time scale (single milliseconds to tens of milliseconds), and that these fluctuations are largely counterion dependent, being especially sensitive to Mg$^{2+}$ concentration. While these fluctuations also occur in the presence of VEGF, results show that the dynamics occur on a slower time scale (hundreds of milliseconds to seconds), indicating that there is indeed an interaction between the aV aptamer and its binding target, VEGF.

R1.00095 Functionalized polymeric nanotubes. CECILE MALARDIER-JUGROOT, Royal Military College of Canada — New nanomaterials already play a key role in several emerging technologies such as nanomotors, nanoelectronics and drug delivery. The increased interest in nanotechnology comes from the fact that nanoscale materials have new physical and chemical properties compared to the bulk. Among the methods used to fabricate new nanomaterials, the most successful in producing precise structure, is the bottom-up method which builds the desired products from the atomic or molecular scale by self-assembly. We will present a new self-assembly process of amphiphilic alternating copolymers into nanotubes combining a computational (molecular modeling) and experimental (small angle neutron scattering, atomic force microscopy) characterization. The nanotubes will be illustrated by the association of poly(styrene-alt-maleic anhydride) and the effect of the functionalization of the polymer chain on the forces stabilizing the nanotubes (hydrogen bonds, π − π interactions) will be presented.
R1.00096 A New Design of Coiled-Coil Helix Bundle Peptide-Polymer Conjugates1. JESSICA SHU, CEN TAN, Department of Materials Science and Engineering, UC Berkeley, WILLIAM DEGRADO, Department of Biochemistry and Biophysics, University of Pennsylvania, TING XU, Department of Materials Science and Engineering, Department of Chemistry, UC Berkeley — Coiled-coil helix bundles, a common tertiary motif found in many natural proteins, underpins many structural and catalytic functions of natural proteins. De novo design has shown that the interior of the helix bundle can be tailored to perform well-defined functions, while the exterior dictates the environment in which it is situated. By attaching synthetic polymers to helix bundle-forming peptides, producing peptide-polymer conjugates, the polymer will mediate the interactions between the helix bundle and its environment, enabling the macroscopic self-assembly of the bundles, and potentially, give them function in non-biological environments. We report a novel design of peptide-polymer conjugates, where upon attachment of polymer to the exterior of the helix bundle stabilizes the peptide secondary and tertiary structures and preserves the built-in function of the bundle. This design strategy should be applicable to other coiled-coil peptides and shows great promise as an avenue toward peptide-based biomolecular functional materials.

3 C. Bertozzi and the Molecular Foundry at Lawrence Berkeley National Laboratory

R1.00097 Effects of molecular weight and entanglement on the dispersion of a layer of platelets in a polymer chain matrix1. BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — A stack of thin sheets (a model for clay platelets) is initially placed in a matrix of polymer chains. How does the dynamic polymer chain matrix (purely entropic constraints) affect the dispersion of sheets is the subject of this computer simulation study. A stack of four sheets constitutes the layer with a small initial inter-layer distance on a discrete lattice. A fraction of the lattice sites are randomly occupied by the polymer chains. Both sheets and chains are modeled by the bond-fluctuation mechanism. Coarse-grained chains and platelets interact and execute their stochastic motion via Metropolis algorithm. Dispersion of the sheets is examined by varying the molecular weight of the polymer chains which form the dynamic network, including entanglements. The relaxation time for dispersion increases on increasing the molecular weight. Exfoliation almost ceases in a matrix with chains beyond a certain length.

We thank AFRL for the support.

R1.00098 Numerical Self-Consistent Field Theory of Flat and Curved Polymer Thin Films TANYA L. CHANTAWANSRI, CARLOS J. GARCIA-CERVERA, HECTOR D. CENICEROS, GLENN H. FREDRICKSON, University of California, Santa Barbara — Using self-consistent field theory, we explore the numerical methods and boundary conditions involved in modeling the self-assembly of inhomogeneous polymer thin films deposited on flat and curved substrates. The model is simulated using a fourth-order accurate spectral collocation method first used by Cochran et al. [Macromolecules 2006, 39, 2449-2451] to model bulk polymeric systems, but where we apply finite difference approximations and non-periodic boundary conditions for the film in the direction normal to the substrate. Boundary conditions are employed to model experimentally relevant substrate conditions such as a "neutral" or attractive bounding surface. For a neutral surface where the substrate has no preferential attraction to either polymer segment, it is appropriate to utilize Neumann boundary conditions, while a surface with a preferential attraction can be modeled using Robin's or mixed boundary conditions.

R1.00099 Topologically constrained polymer collapse, ALEXANDER GROSBERG, University of Minnesota, THOMAS VETTOREL, KURT KRÉMER, Max Planck Institute for Polymer Research, Mainz, Germany — Linear polymer chains in an equilibrium melt are strongly entangled, and coils strongly overlap. Similarly, collapsed (globular) single chain is strongly self-entangled in equilibrium. It is a fundamental question of polymer physics - what happens if the formation of these entanglements or self-entanglements is either completely prohibited or strongly slowed down (like in a melt of unconcentrated rings, in a gel, etc). We address this question by massive Monte Carlo simulation based on the use of non-local moves which dramatically speed up relaxation while strictly preserving the topology. The effects of topologically supported separation of chains, or parts of the same chain, have far reaching applications ranging from gel collapse, to interphase chromosome territories, to statistics of knots in proteins.

R1.00100 Target Finding Time for Microtubules Interacting with Catastrophe-Suppressing Drugs MITRA SHOJANIA FEIZABADI, Canisius College — Target finding time for microtubules interacting with catastrophe-suppressing drugs is investigated in this study. In the steady state of microtubules interacting with catastrophe-suppressing drugs, two types of microtubules exist, one with drug tips and the second without drug tips. This work shows that microtubules in the first group are slower in finding a target than are those in the second group. This result is consistent with experimental findings.

R1.00101 Stability of Fddd structure in diblock copolymer, MYUNG IM KIM, SATOSHI AKASAKA, TSUTOMU WAKADA, MIKIHIITO TAKEKARA, HIROKAZU HASEGAWA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University — Recently we reported a new bicontinuous microdomain morphology with the symmetry of Fddd space group found in a polystyrene-

R1.00102 Applications

R1.00103 Using radar waves to image subsurface heterogeneities: a case study from Randolph College, VA. TATIANA TOTeva, REEUJ POKHAREL, ARCHANa DATTA, Randolph College — A 2D ground penetrating radar survey at 250 MHz central frequency was conducted on Randolph College's campus, in Lynchburg, VA. The experimental setup consisted of three radar profile lines, each with length of 70 – 100 m. The goals of the project were to image subsurface heterogeneities, and define depth to bedrock. Conventional seismic refraction conducted earlier at the site revealed irregular topography of the subsurface and high degree of uncertainty in the arrival times of the elastic waves. Radar surveys have the potential to provide much higher resolution images. We observed a number of point reflectors and multiple layering of the subsurface soil.

R1.00104 Integrated Detector for Ballistic Electron Emission Luminescence, BIQIN HUANG, JING XU, IAN APPELBAUM, University of Delaware — Ballistic electron emission luminescence (BEEL) uses injected hot electrons to induce interband transitions and light emission in semiconductor collectors. Local hot electron injection and ratering from a scanning tunneling probe can therefore potentially provide a means to image buried luminescent layers. However, a sensitive photon detector is required to compensate for low external efficiency. We have designed integrated a Si photodetector to a GaAs/AIGAAs BEEL structure by UHV thin-film metal wafer bonding. This room-temperature technique overcomes index mismatch and numerical aperture problems associated with far-field detection. We expect this method will make BEEL microscopy generally applicable to the study of buried luminescent layers in light emitting devices based on arbitrary material systems. This work is funded by US DOE.
R1.00105 Reduced Contact Resistance in Quantum Cascade Lasers\textsuperscript{1}, MATTHEW ESCARRA, SCOTT HOWARD, ANTHONY HOFFMAN, CLAIRE GMACHL, Princeton University — Quantum cascade (QC) lasers have shown tremendous potential as powerful and compact mid-infrared light sources. However, improvement in the high-efficiency operation of these devices must be made for their transfer to real-world utilization. The internal, current, voltage, and optical efficiencies all must be maximized. In particular, high voltage efficiency requires minimizing the voltage defect in the quantum design and parasitic voltage dropped elsewhere in the device. The majority of this parasitic voltage lies in the metal-semiconductor contact junctions. To study this contact resistance, we designed and fabricated a QC laser structure without the active lasing region. Rapid thermal annealing (RTA) on this “empty” structure shows a 35.2\% reduction in contact resistance at room temperature, which would correspond with a 7\% improvement in laser wall-plug efficiency. Different annealing conditions were tested in order to optimize this reduction. Varying contact metallization and top growth also holds the potential for further reduction in contact resistance and improvement in QC laser efficiency.

\textsuperscript{1}This work is supported in part by DARPA-EMIL and MIRTHE (NSF-ERC).

R1.00106 Quantum-Dot Photodetectors: High Sensitivity due to Controllable Kinetics\textsuperscript{1}, ANDREI SERGEEV, LI-HSIN CHIEN, NIZAMI VAGIDOV, VLADIMIR MITIN, SUNY at Buffalo — Comparing to the quantum wells, the quantum-dot structures provide more opportunities to control electron kinetics and to optimize operating regimes of quantum-dot photodetectors. At room temperatures, the photoelectron capture in quantum-dot structures is determined by the electron diffusion in the potential of intentionally or unintentionally charged quantum dots. Therefore, the capture time can be drastically increased by a proper choice of the quantum-dot structure and modulation doping. Suppression of capture processes provides longer lifetimes of photoelectrons, thus increasing the photoconductive gain and responsivity. Here we exploit a model of the QD detectors operating at room temperatures and study electron diffusion in the self-consistent field of potential barriers surrounding quantum dots. Using the Monte-Carlo method and analytical evaluations, we investigate photoelectron capture and transit processes as functions of the quantum dot positions, sensor geometry, and external electric field applied. Finally, we calculate the photoconductive gain and discuss the optimal structures and regimes. [1] A. Sergeev, V. Mitin, and M. Stroscio, Physica B 316-317, 369 (2002).

\textsuperscript{1}This work was supported by AFOSR and NYSTAR grants.

R1.00107 Cascaded Emission Regions in 2.4 \(\mu\)m GaInAsSb Light Emitting Diode’s for Improved Current Efficiency , JOHN PRINEAS, JEFF YAGER, Dept. Physics and Astronomy, University of Iowa. JONATHON OLESBERG, Optical Science and Technology Center, University of Iowa, CHUANSHUN CAO, Dept. Physics and Astronomy, University of Iowa, MADHU REDDY, Dept. of Physics and Astronomy, University of Iowa, CHRIS CORETSOPOULOS, Optical Science and Technology Center, University of Iowa — Infrared optoelectronics play an important role in sensing of molecules through characteristic vibrational resonances that occur at those wavelengths. For molecules in aqueous and at room temperature, where optical transitions tend to be broad, the broadband emission of light emitting diodes (LEDs) are well suited for obtaining molecular absorption spectra. The 2-2.6 \(\mu\)m range is an advantageous range for sensing of glucose. Voltages available in batteries and control electronics are limited to much higher voltages than those required to turn on an infrared LED, and moreover have limited current supply. Here, we demonstrate room temperature operation of 5-stage cascaded emission regions in 2-2.6 \(\mu\)m GaInAsSb LEDs. We report three times higher turn on voltage, and nine times improved current efficiency compared to a single stage device.

R1.00108 Surface charge effects on the plasmonic band gap of metallodielectric gratings , IAN FOTI-LANDIS\textsuperscript{1}, PAUL WHITE\textsuperscript{2}, JENNIFER STEELE\textsuperscript{3}, Trinity University — Surface plasmon resonances of both metal nanoparticles and metal surfaces are highly sensitive to changes in their dielectric environment. The changes in surface plasmon resonance due to target molecules binding to the metal have been found to be caused by both a local change in dielectric environment as well as changes in the surface chemistry of the metal. The majority of investigations of these competing effects have primarily been limited to the localized surface plasmon resonances of metal nanoparticles. Here, the effects of surface chemistry on surface plasmons will be investigated using metallodielectric gratings. This periodic geometry supports traveling surface plasmon waves that show a plasmonic band gap in the dispersion relationship when two counterpropagating waves are simultaneously excited. The band gap energy changes in response to chemical functionalization, giving unique information on how the surface chemistry affects the surface plasmon resonance. This work focuses on the effect of charged species as a function of pH.

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R1.00109 Electric field controlled left-handed-materials lens\textsuperscript{1}, S.V. BELY, R.V. PETROV, M.I. BICHURIN, A.V. FILIPPOV, Novgorod State University, Russia, G. SRINIVASAN, Oakland University, MI — Microwave lenses are useful for scanning and multi-beam antennas of radar systems, telemetries, and radio-astronomy of the cm and mm-wave bands. The development of electric and/or magnetic field controlled lenses using magnetoelectric material would facilitate improvement if the antenna technologies. We designed such lenses consisting of metal resonators on dielectric substrates with the control elements made of yttrium iron garnet and PZT. The control is based on the variation of magnetic permeability of the ferrite via the electric potential applied to piezoelectric. It results in change in the parameters of transmitted microwave—beam and focal length of the lens. The lens works in cm-wave band. The gain factor of the lens is 6 dB. Theoretical estimates and optimization of the lens parameters were also carried out.

\textsuperscript{1}Supported by grants from NSF, Russian Foundation for Basic Research and Russian Ministry of Education and Science.

R1.00110 Design, fabrication and FEM simulation of a novel Optical-MEMS sensor\textsuperscript{1}, VAIBHAV MATHUR, JIN LI, WILLIAM GOODHUE, Photonics center, University of Massachusetts, Lowell, PHOTONICS CENTER TEAM — Optical waveguides are used in a variety of telecommunications systems to route, add or drop optical signals from the network. Here a combination cantilever/waveguide structure is proposed as the core element of either a vibration/shock sensor or light modulator. An AlGaAs layered dielectric waveguide is fabricated on GaAs substrates and undercut to form a suspended beam. The suspended AlGaAs waveguide is micro-cleaved to produce cantilever segments of equal or unequal lengths, corresponding to either the same or different fundamental frequencies resonance (as the natural frequency is a function of length). The sample is vibrated using a piezo driver. If the vibration frequency supplied to the chip is near one of the resonances the waveguide becomes periodically misaligned as the cantilever displacement amplitude builds up causing a periodic loss in signal at the output end of the guide. In this work cantilever/waveguide structures are fabricated and a detailed FEM(Finite element method) analysis of the device carried out. Also wave propagation and subsequent optical misalignment simulation is carried out on the FEM based COMSOL Multiphysics Package.

\textsuperscript{1}We would like to acknowledge JPS Associates Inc. for laser cutting the samples.
R1.00111 Automation of analysis of electronic microscope images, GAGIK SHMAVONYAN, State Engineering University of Armenia — Many-sided analysis of multiple images of electronic microscope is a hard and time-consuming process. Besides, the analyses become more actual in the case of distorted, not high quality images of electronic microscopes, i.e. images of scanning tunneling microscope. To increase the accuracy and velocity of analyses a method is suggested, which allows analyzing the surface of semiconductor crystal. The method allows to get information on the position of the atoms of the 1\textsuperscript{st}, 2\textsuperscript{nd} and 3\textsuperscript{rd} crystallographic planes, analyze surface defects and dislocations, differentiate two and more materials on the surface, determine surface reconstruction or atomic structure, etc.

R1.00112 A 100 MHz antenna based on magnetoelectric composite materials\textsuperscript{1}, A.S. TATARENKO, R. PETROV, G. SRINIVASAN, Oakland University, M.I. BICHURIN, Novgorod State University — Results on miniaturization of a 100 MHz-antenna based on magneto-electric composites are presented. A composite with large and equal permittivity and permeability is sought for the task. In such composites both miniaturization and impedance match to free-space are possible. A sample of nickel zinc ferrite and bismuth strontium titanate prepared by the conventional ceramic processing is used. The dipole antenna operating at 100 MHz consists of a composite substrate 220 mm in diameter and 8.5 mm in width and a Cu-strip 6.5 mm in diameter. Antenna characteristics are measured with a vector network analyzer. Scattering parameter data indicates resonance at 98 MHz and an antenna miniaturization factor of 7-10, in agreement with theoretical estimates.

\textsuperscript{1}Supported by a grant from DARPA.

R1.00113 Magnetoelectric Composites for 1.3 GHz Antennas\textsuperscript{1}, R.V. PETROV, A.S. TATARENKO, G. SRINIVASAN, Oakland University, Rochester, MI, M.I. BICHURIN, Novgorod State University, Russia — A microstrip miniaturized antenna based on magneto-electric composite has been designed and characterized. Theoretical estimates of antenna properties are given. To miniaturize UHF antennas, one needs slow-wave topologies and magneto-electric (ME) materials with equal and high permeability and permittivity. Nickel Zinc Ferrites (Ni\textsubscript{1-x}Zn\textsubscript{x}Fe\textsubscript{2}O\textsubscript{4}, x=0-0.5, NZFO) are potential candidates for use as the magnetic phase in the composite since they have high permeability, in the range 4-50, and low magnetic loss tangent. The dielectric phase use is bismuth strontium titanates (Sr\textsubscript{1-\textit{r}}Bi\textsubscript{1.5}TiO\textsubscript{3}, 0.04<\textit{r}<0.25, BST) that have high permittivity and low dielectric loss tangent. A sample with nickel zinc ferrite and 2% BST is used. A microstrip dipole element of 47 mm in length and 2 mm in width is placed on a composite substrate with dimensions 65 x 40 x 2.2 mm\textsuperscript{3}. The other side of the substrate has a metal plate plane. Measurements of transfer scattering parameter S\textsubscript{21} are made. A miniaturization factor of 5-10 is achieved. The miniaturization methodology discussed here is useful for mobile communication platforms, radar systems, and remote-controlled ground based systems.

\textsuperscript{1}Supported by a grant from DARPA.

R1.00114 A magneto-electric composite based microwave phase shifter, M.I. BICHURIN, V.M. PETROV, Novgorod State University, Russia, G. SRINIVASAN, Oakland University, Rochester, MI — Magneto-electric (ME) properties of ferrite-ferroelectric composites arise from their response to elastic and electromagnetic force fields. The unique combination of magnetic, electrical, and ME interactions opens up the possibility of electric field tunable ferromagnetic resonance (FMR) based devices [1]. Here we discuss an ME phase shifter operating in the FMR region at 9.3 GHz. A slot line on a yttrium iron garnet film bonded to lead zirconate titanate (PZT) provides a basis for the phase shifter. The circularly polarized microwave magnetic field of the slot line interacts with the ferrite and causes variation of phase velocity with the controlling magnetic and electric fields. Electrical tuning is realized with the application of a control voltage due to PZT. The estimated phase shift per unit length and unit voltage is to 20 deg/cm kV for a PZT thickness of 0.5 mm. 1 S. Shastry and G. Srinivasa, M.I. Bichuri, V.M. Petrov, A.S. Tatarenko. Phys. Rev. B, 70 064416 (2004). - supported by grants from the Office of Naval Research and the Russian Foundation for Basic Research.

R1.00115 Development of a Capacitive Measurement Apparatus for Steel Alloy Magnetostriiction, CHRISTOPHER L. MILBY, JOSEPH L. WIEWEL, MATTHEW W. BECKNER, Department of Physics, Western Illinois University, MARK S. BOLEY, Dep’t of Physics, Western Illinois University — In our laboratory we have developed steel alloy torque transducers that operate via a magnetoelastic principle, converting applied stress to an external magnetic field signal subsequent to appropriate magnetic pre-conditioning. We have found that linearity, repeatability, and sensitivity of these transducers is highly dependent on the heat treatment to which the steel is subjected, which is severely limited by the minimum hardness coefficients that will be required in the actual technological application such as in a power delivery shaft. In our study, we focused on cases where Rockwell hardness coefficients in the forties or low fifties are expected, using a steel alloy with low nickel and chromium content. Austenitizing temperatures varied from 775 to 870 Celsius, whilst tempering temperatures varied from 205 to 540 Celsius, all in a helium atmosphere. The quenching medium following the austenitizing and tempering processes varied between oil and water. The study showed that a tempering temperature around 425 Celsius resulted in the best linearity and re-zeroing capabilities (repeatability) of the transducers, also corresponding to the least hysteresis. Additionally, water quench reduced sensitivity as compared to oil quench at the same temperature.

R1.00116 Determining Optimal Austenitizing and Tempering Temperatures and Quenching Media for a Steel Torque Transducer, JOSEPH L. WIEWEL, CHRISTOPHER L. MILBY, MATTHEW W. BECKNER, MARK S. BOLEY, Department of Physics, Western Illinois University — In our laboratory we have developed a series of high-stress steel alloy magnetoelastic torque transducers that convert applied stress to an external magnetic field signal. We have found that linearity, repeatability, and sensitivity of these transducers is highly dependent on the heat treatment to which the steel is subjected, which is severely limited by the minimum hardness coefficients that will be required in the actual technological application such as in a power delivery shaft. In our study, we focused on cases where Rockwell hardness coefficients in the forties or low fifties are expected, using a steel alloy with low nickel and chromium content. Austenitizing temperatures varied from 775 to 870 Celsius, whilst tempering temperatures varied from 205 to 540 Celsius, all in a helium atmosphere. The quenching medium following the austenitizing and tempering processes varied between oil and water. The study showed that a tempering temperature around 425 Celsius resulted in the best linearity and re-zeroing capabilities (repeatability) of the transducers, also corresponding to the least hysteresis. Additionally, water quench reduced sensitivity as compared to oil quench at the same temperature.

R1.00117 Liquid Supramolecular NanoStamping (LiSuNS), ARUM AMY YU, Massachusetts General Hospital, FRANCESCO STELLACCI, MIT — The development of high resolution bio-devices has generated a demand for the development of novel printing techniques able to minimize fabrication time and labor. Supramolecular NanoStamping (SuNS) is a stamping method that can copy single-stranded DNA features in a sequence specific way in only three steps: a master containing single stranded DNA features is immersed in a solution of complementary DNA (cDNA) molecules modified with a chemical group at the end (Hybridization). Another substrate is placed onto the hybridized master so that a chemical bond can form between cDNA and the secondary substrate (Contact). The two substrates are then separated by heating or mechanical force and a copy composed of cDNA is left on the secondary substrate (Dehybridization). However, like all other contact printing techniques, SuNS’ efficiency highly depends on the roughness of the substrates used. Here, we present an extension of SuNS, Liquid Supramolecular NanoStamping (LiSuNS). LiSuNS eliminates the need of contact between two solid substrates. Using a liquid prepolymer that is cured after contact, using LiSuNS, we achieved large coverage >10cm\textsuperscript{2}. Moreover, because LiSuNS prints 3-D physical information as well as 1-D chemical information (i.e DNA sequences), it can be used to generate a complete DNA-based bio-device with 3-D physical shape (e.g. channels) and chemically modified patterns.
The nanoparticles were exposed to soft x-rays of varying energy under ultra high vacuum, ∼\textit{(adsorbates)}, and we will describe our work to chemically modify the channel in order to control the surface scattering. (NTFETs), even at temperatures approaching 300 K. RTS arises from the population and depopulation of energy levels associated with charge traps along the channel and generate subwavelength patterns. Far-field origins were observed. We present a straightforward model for interference effects generated in our process, and discuss our ability to tune these effects with the fifth harmonic (213 nm) of an Nd:YAG source through metallized contact apertures in contact with resist. Interference patterns with both near- and far-field origins were observed. We present a straightforward model for interference effects generated in our process, and discuss our ability to tune these effects.

In this poster presentation, we discuss opportunities for direct-write UV photolithography through metallized apertures defined by focused ion beam on SPM cantilevers. This process offers subwavelength (<200nm) feature sizes without the need to generate a mask, and the writing process can take place in fully ambient conditions. In our preliminary work, we have patterned polymethyl methacrylate (PMMA) resist by exposing it with the fifth harmonic of a Nd:YAG laser. Experimental results show that the wavelength drift per milliampere of the VCSEL is 0.78 nm/mA.

A simple method for determining the wavelength drift of vertical-cavity surface-emitting lasers (VCSELs) has been studied extensively, and a cutoff frequency of 90 kHz constrained by the bandwidth of thermal response was reported. Results reveal that, with the assistance of polarization-selective optical feedback of about -15 dB, the cutoff frequency of the CDPS could be raised to 50 MHz. A set of rate equations was employed to simulate the enhancement of CDPS and to address the interaction of optical feedback with the PS. These results will help to extend the application of CDPS to even higher frequency.

The present spot size for DNA microarrays is on the order of micrometers. However, there is a need for smaller arrays to allow the detection of smaller volumes of analytes. Although, SPM-based techniques are capable of fabricating nanoscale bio-arrays, such fabrication methods are serial in nature and consequently slow and expensive. A recently introduced method, Supramolecular Nanostamping (SuNS) can overcome this problem by replicating DNA microarrays. In SuNS, a master (i.e. a DNA microarray made of DNA features immobilized onto a surface) is hybridized with its complementary DNA molecules terminated with ‘sticky’ ends to form a secondary structure. A secondary surface is then placed onto the hybridized master to allow for bond formation with the ‘sticky ends’ of the complementary DNA. Afterwards, the master and the secondary surface are separated using heat or mechanical forces effectively achieving a replica of the original DNA array. Here, we demonstrate the application of SuNS to DNA nanoarrays proving that SuNS can reproduce DNA arrays with features as small as 14 ± 2 nm spaced 77 ± 10 nm. Moreover, we show that hybridization of these nanoarrays can be detected using AFM in a simple and scaleable way that does not require labeling of the DNA strands.

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R1.00125 First principles study of hydrogen storage in non-transition metal decorated graphitic materials, GYUBONG KIM, Department of Physics, Pohang University of Science and Technology, NOE JUNG PARK, Department of Applied Physics, Dankuk University, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — Hydrogen has been considered an ideal material that can replace fossil-based fuels as its byproduct is simply water without emitting green house gases. Recently, transition metal (TM)-dispersed porous materials have been suggested as plausible candidates for hydrogen storages that possess optimal hydrogen binding characteristics. A serious problem in this approach is that TM atoms tend to aggregate instead of being atomistically dispersed, which results in the deterioration of hydrogen uptake. Here we study the hydrogen adsorption on non-transition metal (NTM) atoms dispersed on graphene using ab initio methods. We observe that the clustering energy of NTM atoms is much smaller than that of TM atoms, which indicates that NTM can be almost free of clustering on graphene. We also study hydrogen adsorption on those NTM atoms to find comparable storage capacity to that in TM dispersed graphene.

R1.00126 Theoretical study of the structural, mechanical, and electronic properties in hydrides, RYOJI SAHARA, BUN TSUCHIYA, HIROSHI MIZUSEKI, SHINJI NAGATA, TATSUO SHIKAMA, YOSHIYUKI KAWAOE, Institute for Materials Research, Tohoku University — Although an understanding of the mechanical behavior such as elastic properties and hardness of hydrides is important for their applications, theoretical studies have received little attention and only recently some progress has been made. In the present study, first-principles calculations have been performed on hydrides of Ti, Zr, and Hf. The elastic properties are estimated as a function of hydrogen concentration. Equilibrium lattice constants and the bulk moduli are estimated using Murnaghan EOS. While, the elastic constants, shear moduli, and Young’s moduli are estimated introducing the strain tensor. The origin of these properties is explained in terms of the changes in the bonding characters as well as cohesive energy. A semi-empirical relationship between the bulk modulus/shear modulus and the Vickers hardness is introduced to predict hardness of these materials from the present first-principles calculation results.

R1.00127 The crystal structure of $^7\text{Li}_2\text{ND}$, MASAMI TSUBOTA, Institute for Advanced Materials Research, Hiroshima University, MAGNUS H. SORBY, Institute for Energy Technology, Department of Physics, SATOSHI HINO, Graduate School of Advanced Sciences of Matter, Hiroshima University, TAKAKI ICHIKAWA, Institute for Advanced Materials Research, Hiroshima University, BJORN C. HAUBACK, Institute for Energy Technology, Department of Physics, YOSHIKICHI KOJIMA, Institute for Advanced Materials Research, Hiroshima University — Recently much attention has been given to reversible hydrogen storage materials possessing high gravimetric capacity. Lithium amide/imide systems are promising candidates. Chen et al.[1] found that a mixture of lithium amide and lithium hydride can reversibly store hydrogen up to 6.5 mass% forming lithium imide ($\text{Li}_2\text{NH}$). Among them, the crystal structure of $\text{Li}_2\text{NH}$ is still controversial. Balogh et al.[2] have reported a cubic structure model. However, this model differs significantly from theoretical structure models. In this work, the crystal structure of the isotopically substituted $^7\text{Li}_2\text{ND}$ has been investigated by powder neutron and synchrotron X-ray diffraction experiments. In our data some peaks, which should be a single peak for cubic symmetry, were obviously split indicating a lower symmetry than cubic for lithium imide. The structure of $^7\text{Li}_2\text{ND}$ will be described. [1] P. Chen et al., J. Phys. Chem. B 107 (2003) 10967. [2] M.P. Balogh et al., J. Alloys Compd. 420 (2006) 326.

R1.00128 Hydrogen Accumulation inside Single-Walled Carbon Nanotubes Encapsulated in a Pd Matrix, A. LIPSON, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana Champaign, C. H. CASTANO GIRELDO, Department of Nuclear Engineering, Missouri University of Science and Technology, B. F. LYAKHOV, E. I. SAUNIN, A. YU. TSIVADZE, A. N. Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences — Palladium metal possesses the unique property of dissociating molecular hydrogen into an atomic form while simultaneously exhibiting high H-diffusivity, while single-walled carbon nanotubes (SWCNTs) have been actively explored during the last decade as an effective hydrogen storage medium. We report a study of hydrogen storage in which electrochemical hydrogen loading of this material provides reproducibly high net capacity of SWCNT (reduced to hydrogen content in the Pd matrix). The synergistic effect has been achieved by encapsulating Single-Walled Carbon Nanotubes in thin Pd layers on a Pd substrate creates resulting from the combination of the Pd and the SWCNTs properties with regards to hydrogen.

R1.00129 Multimetal plasmonic nanomaterials for solar energy harvesting, RAMKI KALYANARAMAN, JUSTIN TRICE, Dept. of Physics, Washington University in St. Louis, RADHAKRISHNA SURESHKUMAR, Energy, Environmental and Chemical Engineering, Washington University in St. Louis, HERNANDO GARCIA, Dept. of Physics, Southern Illinois University in Edwardsville — Efficient broadband solar absorbing coatings could significantly enhance the performance of Si solar cells. Here, we present the design of novel SiO$_x$-based nanomaterial coatings based on multimetal plasmonic absorption. By implementing an efficient homogenization procedure based on the tight lower bounds of the Bergman-Milton formulation [Garcia et al. Phys. Rev. B, 75, 045439 (2007)], we have predicted the absorption coefficient of a quaternary nanocomposite consisting of Cu, Ag, and Au nanospheres embedded in a SiO$_2$ host matrix. A simulated annealing algorithm was used to predict nanocomposite properties (particle size and volume fractions) which result in a broadband absorption (350 - 800 nm) that matches the shape of the solar emission. These results show that novel optical materials can be made from multimetal-dielectric nanocomposites.

1R.K. and R.S. acknowledge support by the National Science Foundation through CAREER Grant No. DMI-0449258 and No. CTS-0335348, respectively.

R1.00130 ABSTRACT WITHDRAWN

R1.00131 Relation between Packing Density and Thermal Transitions of Alkyl Chains on Layered Silicate and Metal Surfaces, HENDRIK HEINZ, University of Akron, RICHARD A. VAIA, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Characterization through experiment and simulation shows that the orientation of the alkyl layers and reversible phase transitions on heating are a function of the cross-sectional area of the alkyl chains in relation to the available surface area per alkyl chain (packing density). On even surfaces, a packing density less than 0.2 leads to nearly parallel orientation of the alkyl chains on the surface, conformational disorder, and no reversible melting transitions. A packing density between 0.2 and 0.75 leads to intermediate inclination angles, semi-crystalline order, and reversible melting transitions on heating. A packing density above 0.75 results in nearly vertical, lattice-like alignment of the surfactants on the surface and no reversible melting transitions. The same principle applies to curved surfaces, taking into account a local radius of curvature and a distance dependent packing density on the surface. The chain length (minimum C10) and interface chemistry have little impact on this behavior but determine chemical functionality and transition temperatures.
R1.00132 Characterization of iPP/CNT PCN through Transmission Ellipsometry1. GEORGI GEORGIEV, Assumption College, YANEIL CABRERA, TUFTS University, MARK CRONIN, CHRISTOPHER ROCHELEAU, Assumption College, BRIAN FEINBERG, PEGGY CEBE, TUFTS University, ASSUMPTION COLLEGE COLLABORATION, TUFTS UNIVERSITY COLLABORATION — Microscopic Transmission Ellipsometry is a fast and efficient technique for studying anisotropic organization in polymers. Polymer Carbon Nanotube Composites (PCNs) are the largest commercial application of carbon nanotubes (CNT) in nanotechnology. Isotactic Polypropylene (iPP) is one of the best model systems to study in this field because iPP/CNT PCNs can form alpha, beta, and gamma crystallographic phases under a variety of crystallization conditions: nonisothermal and isothermal melt crystallization, shear, stress, fiber extrusion, etc. The morphological structure and the orientation of the crystals can also be finely controlled under those conditions. We complement Microscopic Transmission Ellipsometry studies with other techniques: Differential Scanning Calorimetry, X-ray scattering and dielectric spectroscopy.

1. Research supported by: the National Science Foundation, Polymers Program of the Division of Material Research, grant (DMR-0602473) and NASA grant (NAG8-1167).

R1.00133 Effects of Molecule-Electrode Binding on Molecular Junctions, PETER DOAK, Chemistry UC Berkeley, JON MALEN, Mech. Eng, UC Berkeley, KANHYALAL BAHETI, Chemistry UC Berkeley, ARUN MAJUMDAR, Mech. Eng, UC Berkeley, RACHEL SEGALMAN, Chem. Eng, UC Berkeley, DON TILLEY, Chemistry UC Berkeley — Measurements of the Seebeck coefficient or thermopower of metal-molecule-metal junctions offer additional insight into single molecule transport. By applying a temperature bias across a junction created via an Au-Au STM break junction a thermoelectric voltage can be measured which is related to the transmission function through a derivative. Previously dithiol molecules have been studied by this method. Here, the effects of altering the binding to the electrodes will be demonstrated. When the binding group is altered to cyano or amine functionalities, the thermopower is greatly affected suggesting markedly different behavior in response to tuning of molecular energy levels. This indicates important changes in the junction transmission functions near the chemical potential of the contacts. For example, we show that measurements of dinitrile molecules cannot be interpreted as simple shifts of a single Lorentzian transmission peak across the contact chemical potential. Additionally these measurements show that the binding groups can have considerably more influence on junction behavior than other forms of molecular functionalization and provide a useful means to interrogate theories of junction transport.

R1.00134 Controlled one dimensional poly (3-hexythiophene) nano fiber for high performance organic field effect transistor, SUNG WON LEE, UNYONG JEONG, Yonsei University — We demonstrate here how to fabricate cylinder shape, one dimensional organic field effect transistor for high performance field effect transistor device. To reduce the size and increase component density in circuit we used electro-spinning as a fabrication method. Coaxial nozzle was used for cylindrical semiconductor and gate insulator defines. Regio-regular Poly (3-hexythiophene) and poly vinyl phenol was used as semiconductor and gate insulator respectively. Electrical performance is not reported here because of environmental instability. However, we expect good electrical performance will be shown shortly because this device form cylindrical conduction channel compare to thin film type field effect transistor. Here we propose electro-spinning is an easy one step process to fabricate one dimensional polymer field effect transistor.

R1.00135 Low-temperature characterization of organic conducting thin films, GREGORY TOPASNA, DANIELA TOPASNA, Virginia Military Institute — Conducting polymer thin films were investigated at low temperatures. We present results for such a spin coated film made of poly[2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene] (MEH-PPV) which was tested for temperatures below 20 °C. The film was probed over several cycles of cooling then heating. For each cycle the results showed a similar temperature dependent resistance. Such polymer thin films have potential applications as flexible temperature sensors.

R1.00136 Electronic properties of adjoined TiO2 nanocrystals1, O. DIWALD, M.I. ELSER, N. SIEDL, Vienna University of Technology, Institute of Materials Chemistry, J. BERNARDI, Vienna University of Technology, USTEM — The discussion of particle attachment effects is indispensable for deeper insights into electronic conduction across grain boundaries and thus essential to photovoltaics. We investigated the condensation of isolated TiO2–nanocrystals [1] induced via the application of a simple hydration-dehydration cycle. The resulting particle network shows a mesoporous structure as well as significant changes in the optical absorption properties as investigated by UV-diffuse reflectance spectroscopy. In addition, polarizable conduction band electrons are only observed in the network which consists of adjoined TiO2–nanocrystals [2]. Since photo-assisted tunneling between localized states in the oxide particle network represents an important conduction mechanism in dye-sensitised solar cells, UV induced charge separation processes were studied on nanocrystal aggregates using EPR and IR spectroscopy. Corresponding results will be discussed in the light of associated structural data. [1] Berger et al. Chem. Phys. Chem. 2005 6 2104-2112 [2] Elser et al. J. Phys. Chem. B 2006, 110, 7605

1. Financial support from the Austrian Fonds zur Foerderung der wissenschaftlichen Forschung (P19702-N20) is gratefully acknowledged.

R1.00137 Photooxidation of Acetone and Butanone on Rutile TiO2 (110)2, DANIEL P. WILSON, DAVID SPORLEDER, Stony Brook University, MICHAEL G. WHITE, Stony Brook University, Brookhaven National Laboratory, WHITE GROUP TEAM — Interest in the photooxidation of organic compounds on heterogeneous surfaces such as TiO2 has increased in recent years. Here, acetone and butanone, two common organic ketones, are studied under UHV conditions to determine what fragmentation occurs during photooxidation and to gain insight as to the predictability of desorbing species. The data was collected using a pump-probe time-of-flight (TOF) method. Excitation occurs via exposure to 3.7 eV photons followed by ionization with 13.05 eV photons. Preheating the surface to ~200K facilitated the formation of an organic-diatole species needed for photoactivity. During butanone photooxidation, different desorption mechanisms between mass 30 and masses 27-29 are evident. Background thermal results and preliminary translational energy distributions are calculated for acetone and some butanone fragments and are presented here.

2. Acknowledgments: This work is supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences under contract DE-AC02-98CH10866.

R1.00138 Ultrafast Carrier Dynamics in Water-Splitting Photocatalysts, ELIZABETH CARROLL, OWEN COMPTON, MICHAEL SARAHAN, FRANK OSTERLOH, DELMAR LARSEN, Department of Chemistry, University of California — Semiconductors that photocatalytically split water into hydrogen and oxygen using solar energy represent promising renewable energy technologies. Charge carrier dynamics on sub-nanosecond timescales dictate the overall efficiency of charge separation, and consequently, photocatalytic activity of these materials. Using transient absorption spectroscopy, we investigated photoexcited carrier trapping, recombination, and interfacial charge transfer dynamics in water-splitting niobate nanosheets. Ca2Nb2O10 generated H2 from water with 0.22% quantum yield, but no O2 was formed. Carriers relaxed with second-order kinetics on a sub-nanosecond time scale that depended on the nanosheet size. Methanol was used as a sacrificial donor to separate electron and hole dynamics and identify absorption spectra for the trapped carriers. In aqueous methanol, hole scavenging was observed within 100 ps in direct competition with electron-hole recombination. The nanosheets were also functionalized with metal and semiconductor nanoparticles to form novel photocatalyst nanostructures. Colloidal IrO2 was attached to Ca2Nb2O10 to sensitize the catalyst for visible light absorption. Interfacial electron transfer stabilized the charge separation in IrO2, and O2 was generated.
Part of this presentation was supported by the Louisiana Department of Natural Resources through a grant with the U.S. Department of Energy.

R1.00139 Applications of Physics to Measuring and Improving the Performance of Buildings in Hot, Humid, Hurricane-Prone Climates1, NORMAN WITRIOL2, Building Science Innovators and The Regen Group, MYRON KATZ, NOLA Solar, Building Science Innovators and The Regen Group, CHRISTOPHER FAUST, NOLA Solar and The Regen Group, JINSION ERINJERI, Louisiana Tech University — In this presentation we will present topics showing how physics can be applied to measuring and improving the performance (energy efficiency and durability of the structure, health, safety, and comfort of the occupants) of buildings in hot, humid, hurricane-prone climates representative of the climate in New Orleans and the Gulf Coast.

1Retired, Louisiana Tech University

R1.00140 Modeling of Magnetic Field Assisted Assembly, RENE RIVERO, SHAMMUGAMURTHY FNU, GAURAV DEVRAHI, VIJAY KASISOMAYAJULA, MICHAEL BOOTY, ANTHONY FIORY, NUGGHELLI RAVINDRA, New Jersey Institute of Technology — A simplified model of the magnetic field assisted assembly process is presented and developed. Objects are moved by magnetic forces into an assembled pattern such as into an array of recesses. All the forces involved in the assembly process are considered in the model. An example in which an object comes in contact with the recess and settles into it in order to initiate the modeling process is illustrated. Experimental techniques for the assembly process with an optimal control system with feedback is described. The results of the study are analyzed in relation to applications in fabricating heterogeneous systems.

R1.00141 Probing molecules in integrated silicon-molecule-metal junctions by inelastic tunneling spectroscopy, WENYONG WANG, National Institute of Standards and Technology, ADINA SCOTT, Purdue, NADINE GERGEL-HACKETT, CHRISTINA HACKER, NIST, DAVID JANES, Purdue, CURT RICHTER, NIST — A hybrid technology where molecular devices are integrated with traditional semiconductor microelectronics is a promising approach for future electronic applications. Key challenges in this area include developing devices in which the molecular integrity is preserved and defining in-situ characterization techniques to probe the molecules within the completed devices. In this study, we present the first experimental report of inelastic electron tunneling spectroscopy of integrated metal-molecule-silicon devices with molecules assembled directly to silicon contacts. The results provide direct experimental confirmation that the chemical integrity of the monolayer is preserved and that the molecules play a direct role in electronic conduction through the devices. Spectra obtained under varying measurement conditions show differences related to the silicon electrode, which can provide valuable information about the physics influencing carrier transport in these molecule/Si hybrid devices.

R1.00142 Watching electrons tunnel, SIMON MOSER — To get insight to time resolved inner atomic or molecular processes, laser pulses of few femtoseconds or even attoseconds are needed. These short light pulse techniques ask for broad frequency spectra, control of dispersion and control of phase. Hence, linear optics fails and nonlinear optics in high electromagnetic fields is needed to satisfy the amount of control that is needed. One recent application of attosecond laser pulses is time resolved visualization of tunnel ionization in atoms applied to high electromagnetic fields. Here, Ne atom electrons are excited by an extreme ultraviolet attosecond laser pulse. After a while, a few cycles nearly infrared femtosecond laser pulse is applied to the atom causing tunnel ionization. The ion yield distribution can be measured as function of the delay time between excitation and ionization and so deliver insight to the time resolved mechanisms.

R1.00143 Application of the double and triple parabolic quantum well in a laser, MARTIN MOLINAR, GERMAN CAMPOY, Departamento de Investigacion en Fisica, Universidad de Sonora — Using a structure of two and three consecutive parabolic potentials (harmonic oscillator), enclosed in an infinite rectangular well, we solve the Schroedinger’s equation and get the eigenvalues for the Hamiltonian. Trying with a few periods of the structure, we can see the rise of subbands. This system can be used for the development of a semiconductor laser diode built with the deposition of semiconductors on a substrate. We calculate the energy differences between neighboring states and they are then compared with those values found in the literature for similar systems. The emission frequency, the gain and the efficiency of the periodic structure are calculated, for different widths of the parabolic wells and this let us to explore the possibility of use parabolic potentials instead rectangular wells for build a semiconductor laser diode.

R1.00144 ATOMIC, MOLECULAR & OPTICAL (AMO) PHYSICS –

R1.00145 Making BEC for study Quantum physics by modulating the Magnetic potential, JINAH PARK, DAHYUN YUM, WONHO JHE, Department of Physics and Astronomy, Seoul National University — The achievement of Bose Einstein Condensation (BEC) has opened a new chapter in atomic physics. With BEC in dilute atomic gases, quantum physics, solid state physics modeling and many physical phenomena, which has been hard to treat, could be studied beyond the research on BEC itself. In this sense, BEC in ultracold weakly interacting gases has been a very important meaning in recent years. Until now, many experimental results related with thermal atoms in the modulating potential have been carried out. It is no doubt that it is very interesting subject to study quantum mechanical phenomena in various potential configurations. We have been experimenting with the neutral rubidium 87 atoms for making BEC. Our experimental setup to obtain BEC is consisted of double Magneto-Optical Trap (MOT) system, Time Orbiting Potential (TOP) magnetic trap and evaporative cooling technique using rf-knife edge which is typical BEC setup. Here our experimental results are reported.

R1.00146 Superconducting atom chips: recent results and prospects, ADRIAN LUPASCU, CEDRIC ROUX, ANDREAS EMMERT, THOMAS NIRRENGARTEN, GILLES NOGUES, MICHEL BRUNE, JEAN-MICHEL RAIMOND, SERGE HAROCHE, Kastler-Brossel Laboratory, Ecole Normale Superieure (Paris) — Atom chips offer a very interesting set of tools for the magnetic trapping and manipulation of neutral atoms close to surfaces and on-chip optoelectronic devices. In our experiments we investigate atom chips built using superconducting wires in a cryogenic environment. We have recently produced the first Bose-Einstein condensate using this setup. We observe the onset of the Bose-Einstein condensation for 1 x 10^5 atoms at a temperature of 100 nK. This result opens the way for studies of ultra-cold atoms interacting with superconducting structures. We also envision to excite the dense atomic cloud towards long lived Rydberg states. Making use of the phenomenon of dipole blockade could lead to the deterministic production of a single atom in a Rydberg state.

1 Funded by the National Science Foundation

R1.00148 Bose-Einstein condensation in low dimensional layered structures1. PATRICIA SALAS, Posgrado en Ciencia e Ingeniería de Materiales, UNAM, Mexico, M.A. SOLIS, Instituto de Física, UNAM, Apartado Postal 20-364, Mexico, D.F., Mexico — Bose-Einstein condensation critical temperature, among other thermodynamic properties are reported for an ideal boson gas inside layered structures created by trapping potential of the Kronig-Penney type. We start with a big box where we introduce the Kronig-Penney potential in three directions to get a honey comb of cubes of side a size and walls of variable penetrability ($P=mVab/h^2$), with bosons instead of bees. We are able to reduce the dimensions of the cubes to simulate bosons inside quantum dots. The critical temperature, starting from that of an ideal boson gas inside the big box, decreases as the small cube wall impenetrability increases arriving to a tiny but different from zero when the penetrability is zero ($P \rightarrow \infty$). We also calculate the internal energy and the specific heat, and compare them to the ones obtained for the case of the same Kronig-Penney potential in one direction (simulating layers), and two directions (nanotubes).

1 We acknowledge the partial support from grant PAPIIT IN111405-3 and CONACYT 43234-F.

R1.00149 Spin Nematics and Quantum Fluctuation-Controlled Coherent Spin Dynamics of Hyperfine Spin F=2 Cold Atoms1. JUN LIANG SONG, GORDON SEMENOFF, FEI ZHOU, The Univ. of British Columbia — We show that quantum fluctuations lift the accidental continuous degeneracy that was found in the mean field analysis of spin nematic states of hyperfine spin F=2 87Rb. Two distinct spin nematic states with higher symmetries are selected out depending on scattering lengths: a uniaxial spin nematic and a biaxial spin nematic. Recently we also study coherent spin dynamics mainly driven by quantum fluctuations. Unlike the usual mean-field driven dynamics, quantum fluctuation-controlled spin dynamics are sensitive to the variation of fluctuations and the potential induced by quantum fluctuations can be tuned by four or five orders of magnitude in optical lattices. These dynamics have unique dependence on quadratic Zeeman fields and potential depth in optical lattices. We find that although these dynamics are difficult to observe in traps, it is possible to observe them in optical lattices; particularly they can survive in F=2 87Rb condensates with a relatively short life time.

1 This work is supported by the office of the Dean of Science, University of British Columbia, NSERC(Canada), Canadian Institute for Advanced Research, and the Alfred P. Sloan foundation.

R1.00150 Bose-Einstein Condensates of Cesium Atoms in an Optical Lattice1. CHEN-LUNG HUNG, XIBO ZHANG, NATHAN GEMELKE, CHENG CHIN, University of Chicago — The realization of the Mott-insulator to superfluid phase transition with neutral atoms in an optical lattice provides a rare opportunity to test many-body physics with accuracy. We report progress on an experimental and quantitative comparison of the superfluid to Mott-insulator phase boundary with results from the Bose-Hubbard model, using Bose-condensed cesium atoms confined to a thin layer of an optical lattice potential. Feshbach resonances with cesium atoms enable us to scan the on-site interaction over a wide range without modifying the tunneling rate and the overall trapping potential; chemical potential can be adjusted by loading a varied mean atomic density into the lattice. We describe the physical apparatus constructed for this investigation, including novel construction designed to achieve precise and agile control of the magnetic field used in tuning interactions, adiabatic loading and manipulation of the lattice potential, and tight two-dimensional confinement applied to negate the effect of gravity without sacrifice in system homogeneity. 

1 We acknowledge support of MRSEC and Packard, Grainger and Sloan Fellowships.

R1.00151 Development of an apparatus for simultaneous trapping of 6Li—87Rb mixtures. QUN WEI, MICHAEL BROWN-HAYES, WOO-JOONG KIM, Dartmouth College, CARLO PRESILLA, University of Rome “La Sapienza” and INFM-CNR, ROBERTO ONOFRIO, Dartmouth College and University of Padova — Ultracold dilute atomic gases are providing a new window into quantum physics, with particular regard to the first-principle study of various superfluid phenomena. It is critical, in order to open this window, to reach deeper Fermi degeneracy, and this requires, for Fermi-Bose mixtures, to optimize the heat capacity matching between the Fermi and the Bose gases. After discussing a thermodynamic model showing that heat capacity matching is improved by using species selective traps, we discuss the status of an apparatus in which we trap fermionic 6Li and bosonic 87Rb in a magneto-optical trap.

R1.00152 Casimir forces in sphere-plane and cylindrical-plane geometries. QUN WEI, WOO-JOONG KIM, MICHAEL BROWN-HAYES, Dartmouth College. DIEGO DALVIT, Los Alamos, HAYDEN BROWNELL, ROBERTO ONOFRIO, Dartmouth College — We report on the status of an experiment aimed at measuring the Casimir force in cylinder-plane geometry. In order to characterize the apparatus, we have first performed small distance electrostatic calibrations in the sphere-plane geometry free from parallelism issues. This has allowed us to better identify various general issues on the measurement of the Casimir force, such as the distance dependence of the residual (contact) potential, and the delicate assessment of the absolute distance. Recent electrostatic calibrations in the cylinder-plane geometry after an upgrade of the parallelization system will be also reported.

R1.00153 Universal Dependence in Ultra-Cold Fermi Gases. SHIZHONG ZHANG, Department of Physics, University of Illinois at Urbana-Champaign — Over the last few years, there have been considerable efforts in understanding the physics of BEC-BCS crossover in ultra-cold fermi gases. Despite the fact that the problem can be easily formulated, it has not been amendable to analytic solutions. Various approximations have been used to address the problem especially around unitarity. Here we present some general considerations on the problem, relying on the fact that the system is dilute and thus the interaction effects comes only from two-body encounters. These enables us to express certain physical quantities(total energy, interaction energy, rf-spectroscopy shift and closed channel fractions) in terms of one universal function, depending only on temperature and interaction strength. The result obtained should be valid throughout the crossover and thus we expect it to have testable consequences in the future experiments.
R1.00154 Ultra-cold atom experiment and strongly interacting Fermi system. LI YAN, Stony Brook University, STONY BROOK COLLABORATION — Recent progresses in low temperature atomic experiment, especially the magnetic tunable inner-atom interaction via Feshbach resonance, give people a way to approach the study of low temperature and strongly interacting fermion system. In the strong interaction limit, i.e. the unitary limit range, system experiences BCS-BEC crossover, with universal thermodynamic properties. This kind of universality not only simplifies the theoretical research on strongly interacting fermion system but also help people to prove the uniqueness of strongly interacting system in ultra-cold atom experiment.

R1.00155 Emergent vortex dynamics in two-dimensional neutral superfluids. CHENG-CHING WANG, Dept. of Physics, Univ. of Texas at Austin, REMBERT DUNE, Inst. for Theoretical Physics, Utrecht University, MACDONALD ALLAN, Dept. of Physics, Univ. of Texas at Austin — We derive an effective action for the vortex translational zero modes of a superfluid by integrating out environmental modes which include phase and density fluctuations of the condensate. When the quantum dynamics of the fluctuations are treated as frozen with negligible Berry phases in adiabatic limit, we confirm the occurrence of vortex Magnus force and adiabatic vortex mass due to compressibility of the superfluids in agreement with earlier studies. In addition, we also show the results beyond adiabatic limit in which the quantum dissipative action can be derived and solved analytically. We show that the adiabatic approximation is only valid in large system with small coherence length $R \gg \xi$. Furthermore, we also build a numerical model based on discrete Gross-Pitaevskii equation to show the renormalization and broadening of the vortex cyclotron resonance peaks. It is demonstrated that well-defined cyclotron peaks in spectral functions can be sustained only when the condition $R \gg \xi$ is satisfied. With the mapping between discrete Gross-Pitaevskii equation and bosonic single-band Hubbard model, we propose that the adiabatic vortex dynamics can be realized by tuning the ratio between tunneling energy $J$ and on-site interaction energy $U$ such that $U N_a \gg J$ in cold atom systems with optical lattices, in which $N_a$ is the total number of bosonic atoms.

R1.00156 Violation of classical inequalities and EPR correlations in a two-mode three-level atomic system. EYOB SETE, New Mexico State University — We investigate violation of Cauchy-Schwarz and Bell inequalities in two-mode three-level atomic system show that this system can be used to prepare states that exhibits EPR correlations.

R1.00157 Fiber optic laser delivery system for planar ion traps. ELIZABETH GEORGE, DAVID LEIRANDT, ISAAC CHUANG, MIT — The use of trapped ions for quantum computation requires precise focusing and alignment of lasers for cooling the ions and performing logic gates. On-trap fiber optics would eliminate the need for alignment of lasers to the traps and allow scaling of surface-electrode ion traps on large chips to smaller sizes. We have developed a design for implementing on-trap fiber optics with an integrated beam focusing lens using microfabrication techniques. The design uses SU-8 photoresists structures to align the fiber and focusing lens to the trap. We present details of the design and the results of preliminary testing.

R1.00158 In-Situ Optical Heterodyne in time Resolved Coherent Anti-Stokes Raman Scattering. YEHIAHM PRIOR, ANDREY SHALIT, YURI PASKOVER, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — We show both theoretically and experimentally that pure vibrational modes cannot be observed in the power spectrum of time resolved degenerate Coherent anti-Stokes Raman Scattering (CARS), unless the optical signal is linearized by an optical heterodyne detection scheme. A new heterodyne detection method is introduced, where the local oscillator is not provided externally, but is produced in-situ by the addition of small amounts of highly anisotropic molecules to the measured sample. The rotational anisotropy of the added molecules gives rise to a slowly evolving signal, which in turn serve as the local oscillator in heterodyned time resolved CARS. We have shown that the strength of the local oscillator can be controlled by amount of material added, in our experiments $C_3$ added to the measured chloroform or bromoform liquids. Small change of total anisotropy of the sample is expressed as dramatic changes in the intensity of the peaks corresponding to the fundamental vibrational frequencies. This method can be utilized for distinguishing of the fundamental frequencies from beats appearing in the signal due to quadratic (intensity) detection of the nonlinear signal.

R1.00159 Cold antiproton production in the ATRAP2 apparatus. JONATHAN WRUBEL, G. GABRIELSE, P. LAROCHELLE, D. LE SAGE, B. LEVITT, W.S. KOLTHAMMER, R. MCCONNELL, P. RICHERME, A. SPECK, Harvard University, M.C. GEORGE, D. GRZONKA, W. OELERT, T. SEFZICK, Z. ZHANG, Forschungszentrum Julich GmbH, A. CAREW, D. COMEAU, E.A. HESSELS, C.H. STORRY, M. WEEL, J. WALZ, Institut fur Physik, Mainz, ATRAP COLLABORATION — We have developed a new ATRAP2 experimental platform, which has succeeded in producing thousands of anthydrogen ($\bar{H}$) atoms in a combined Penning-Ioffe trap. The Penning trap provides confinement for charged particles needed for future laser cooling and precision spectroscopy of $\bar{H}$. As the $\bar{H}$ atoms are formed that by the addition of small amounts of highly anisotropic molecules to windows in the Ioffe trap to transmit Lyman-$\alpha$ radiation into the production space, which is needed for future laser cooling and precision spectroscopy of $\bar{H}$.

R1.00160 Density Matrix Descriptions for Pump-Probe Optical Phenomena in Moving Atomic Systems1, VERNE JACOBS, Naval Research Laboratory — Reduced density matrix descriptions are developed for pump-probe optical phenomena in moving many-electron atomic systems, taking into account atomic collisions and external magnetic fields. Time-domain (equation-of-motion) and frequency-domain (resolvent-operator) formulations are developed in a unified manner. In a semiclassical perturbative treatment of the electromagnetic interaction, compact Liouville-space operator expressions are derived for the linear and the general ($n$th order) non-linear electromagnetic-response tensors. These expressions are valid for coherent atomic excitations and for the full tetradic-matrix form of the collision operator in the Markov approximation.

R1.00161 Ab initio studies on molecules and clusters in external electrostatic fields. RAJEEV PATHAK, Department of Physics, University of Pune, Pune 411007, Maharashtra, India — Influence of a uniform static external electric field on some aliphatic and aromatic molecular species is studied within the density functional theory (DFT) employing the 6-311++G(2d,2p) basis-set with B3LYP exchange-correlation prescription. The electric field perturbs the molecular geometry; alters the dipole moments and engenders a molecular vibrational Stark effect. For polar molecules, significant frequency shifts are observed for field orientations both parallel and antiparallel to their permanent dipole moments; where HOMO-LUMO gaps alter significantly. Time dependent DFT analysis reveals that an increase in the applied field strength increases the excitation energies amongst frontier MOs with a concomitant decrease in oscillator strengths. Structural evolution of water clusters, ($H_2O)_n$, $n=6-8$ is studied within DFT: the intermolecular hydrogen bonds stretch, and eventually break at some threshold values, triggering a conformational transformation, with configurations appearing as local minima on the cluster’s potential energy landscape, with abrupt increase in the electric dipole moments and ‘opening up’ of three dimensional morphologies of water.
R1.00162 Analysis of the nuclear motion in a HeNe* transient molecule. CRISTIAN BAHRIM, JOSEPH HUNT, Department of Chemistry and Physics, Lamar University - Texas — Based on a model potential for describing the interaction between He and Ne* atoms during a collision [1] we predict a series of vibrational states within several electronic adiabatic potential wells of the HeNe* system for internuclear distances \( R < 6 \, \text{a}_0 \). The identification of vibrational states suggests the formation of a HeNe* transient molecule. In our study two theoretical approaches are employed: (1) the harmonic approximation is based on the assumption that during a collision (which is considered as being one period of vibration) the nuclear motion is harmonic, and (2) the anharmonic approximation which uses the best fit of the electronic adiabatic potential wells with a Morse anharmonic function, as is typically done for stable molecules [2]. A set of vibrational-electronic transitions which can be measured using IR spectroscopy is proposed. The relative population of Ne* atoms after collisions and various IR photo-absorption is predicted for experimental testing of the dominant character of the nuclear motion: whether harmonic or anharmonic. The existence of a HeNe* transient molecule could have a positive impact on improving the performance of He-Ne lasers. [1] Bahrim C, Kucal H and Masnou-Seeuws F 1997 Phys. Rev. A 56 1305. [2] Bahrim C and Hunt J 2006 J. Phys. B 39 4683.

R1.00163 Compton Profiles of Atoms and Ions. KHONDKAR KARIM, Illinois State University — We present momentum-space properties of several atoms and ions including He, Be, B, C, N, O, and Ne atoms, and the respective ions in many possible ionization stages. The calculations have been done using Hartree-Fock atomic models. The Compton profile data presented here could be used to obtain doubly differential cross section of electron production in ion-atom collision from electron-ion cross sections. The plots of electron distribution in momentum space reveal interesting features that are not apparent in electron’s radial probability distribution in coordinate space.

R1.00164 Fully Differential Cross Sections in Two-Photon Double Ionization of Helium. DANIEL HORNER, Theoretical Division, Los Alamos National Laboratory; THOMAS RESCIGNO, Chemical Sciences, Lawrence Berkeley National Laboratory; C. WILLIAM MCCURDY, Chemical Sciences, Lawrence Berkeley National Laboratory; Applied Science and Chemistry, U. California, Davis — We present total, single differential, and triple differential cross sections for two-photon double ionization of helium above and below the threshold for sequential ionization (54.4 eV). Sequential double ionization exhibits characteristic behavior seen in the total and differential cross sections. Evidence of this behavior also arises below the threshold through “virtual sequential ionization.” Using the method of exterior complex scaling, we compute numerically converged wave functions describing two unbound electrons on a large, but finite volume. From these wave functions, using formally exact integral methods, we extract ionization amplitudes, from threshold through “virtual sequential ionization.”

R1.00165 Adsorbates Effects in H−Na/Cu(111) collisions. BOGDANA BAHRIM, SONG YU, Department of Chemistry and Physics, Lamar University - Texas — The (111) faces of Cu, Ag and Au present a band gap that extends just below the vacuum level at the \( \Gamma \)-point [1]. The effect is to forbid electrons with energies in a certain range to be transferred into the metal along the surface normal. Thus, the presence of a band gap should dramatically influence various experiments in ion-surface collisions involving electron capture or loss. In recent years, this topic received a great interest [2 – 4]. Adsorbates deposition makes the electron dynamics at such surfaces to be even more complex. We analyze some interesting adsorbates of a band gap should dramatically influence various experiments in ion-surface collisions involving electron capture or loss. In recent years, this topic received a great interest [2 – 4]. Adsorbates deposition makes the electron dynamics at such surfaces to be even more complex. We analyze some interesting adsorbates of a band gap should dramatically influence various experiments in ion-surface collision with various ions in the target.

R1.00166 Spectroscopic and Magnetic Susceptibility Analyses of the \( \text{F}_J \) and \( \text{D}_4 \) Multiplet Manifolds of Tb\( ^{3+}(4\text{f}^8) \) in TbAlO\(_3\). KELLY NASH, JOHN GRUBER, DHIRAJ SARDAR, University of Texas at San Antonio, UYGUN VALIEV, ABDULLA UZOKOV, National University of Uzbekistan, GARY BURDICK, Andrews University — Detailed analyses of temperature-dependent spectroscopic and magnetic susceptibility data are reported for the crystal-field split energy levels of the \( \text{F}_J \) and \( \text{D}_4 \) of Tb\(^{3+}\) in TbAlO\(_3\). The spectroscopic data include absorption spectra obtained between 460 and 2920 nm from 8 to 300 K. High resolution fluorescence spectra are reported, representing transitions from \( \text{D}_4 \) to \( \text{F}_5 \) at a sample temperature of 85 K. Using crystal-field modeling techniques recently adapted for low symmetry systems, we have assigned all 5 experimental Stark levels within the \( \text{F}_J \) and \( \text{D}_4 \) manifolds, with a fitting standard deviation of 4.5 cm\(^{-1}\) (3.8 cm\(^{-1}\) rms error). Furthermore, the theoretical Stark levels and calculated wavefunctions were used to determine the temperature dependence of the magnetic susceptibility along the c-axis of the TbAlO\(_3\) crystal. Agreement is obtained between the calculated susceptibility and temperature-dependent magnetic data reported earlier. The susceptibility calculation also confirms the predicted ordering of states within the \( \text{F}_6 \) multiplet manifold.

R1.00167 Ultracold Cesium Feshbach Molecules. MICHAEL MARK, STEVEN KNOOP, FRANCESCA FERLAINO, MARTIN BERNINGER, HARALD SCHÖBEL, HANNS-CHRISTOPH NÄGERL, RUDOLF GRIMM, University of Innsbruck, Austria — We present our recent work on ultracold Cesium Feshbach molecules in an optical dipole trap. We have implemented a new crossed-beam laser trap, which traps atoms and molecules simultaneously. By scanning one laser beam the ellipticity can be dynamically tuned for an optimal trap configuration. We routinely prepare ultracold mixed atomic and molecular or pure molecular samples at temperatures down to 30 nK [1]. We selectively populate Feshbach molecules in various \( s-, d-, q- \) and \( q- \) l-wave states [2]. We have experimentally demonstrated that the \( q- \) dimers can be stable against spontaneous decay on the timescale of one second well above the dissociation threshold [3]. We have recently implemented the technique of resonantly modulated magnetic field spectroscopy [4]. Transitions between the atomic continuum and dimer states, and vice versa, as well as dimer-dimer transitions can be driven. Our main motivation is to apply this technique to search for trimer and tetramer states, whose presence has been indicated by resonances in collisional loss measurements.

R1.00168 Helium Spectra in Atomic Mechanics. ALFRED PHILLIPS, JR., SOURCE INSTITUTE — In our model of the helium atom, we postulate that the angular momentum of each electron divided by \( h \) equals an integer, \( n \), plus a fraction, \( \Delta n \). By minimizing the energy the energy of the helium atom, we find that the \( \Delta n \) values are a function of the total angular momenta, \( J \), irrespective of the integer, \( n \). We thus obtain a set of \( \Delta n \) values for the singlet and triplet states of helium. The \( \Delta n \) values are related to fractals. In our model, we made adjustments to the electron mass so that the calculated energy values agree with the seventeen values for the singlet \( ls \)-ns configurations listed in NIST Atomic Spectra Database Levels Data. The adjustments to the electron mass were very close to unity except for the ground state for which the adjustment was \(-5\%\). (Adjustments like these suggest that we may be able to study three-body effects with spectral accuracy.) By doing this, we had good agreement with all of the NIST spectral values for helium (191 lines of He I, and 243 lines of He II). This conceptually and mathematically simple procedure can be used for other atoms.
R1.00169 The Adiabatic-to-Diabatic Mixing Angle for the Inelastic Collision \( B(2P_{1/2}) \rightarrow H_2(j, n) \leftrightarrow B(2P_{3/2}) + H_2(j', n') \)

DAVID WEEKS, MATTHEW GARVIN, Air Force Institute of Technology — The Born-Oppenheimer approximation breaks down when two adiabatic potential energy surfaces become sufficiently close. Under these conditions, the nuclear dynamics are governed by a set of coupled diabatic surfaces. Derivative coupling matrix elements can be used to compute the transformation from the adiabatic to the diabatic potential energy surfaces. A line integral along various contours through the vector field defined by the derivative coupling matrix elements is used to compute the adiabatic-to-diabatic mixing angle. In particular, we investigate the path independence of this coupling angle for the inelastic collision \( B(2P_{1/2}) + H_2(j) \rightarrow B(2P_{3/2}) + H_2(j') \) collision (1). (1) D.E. Weeks, T.A. Niday, and S.H. Yang, J. Chem. Phys. 125, 164301 (2006).

R1.00170 Vibrational and Spin as well as Linear Kinetic Energies Should Be Included in Pair Production and Annihilation Energy Relations

STEWART BREKKE, Northeastern Illinois University (former grad student) — By including the vibrational and spin kinetic energies in Pair Production and Annihilation Formulas a closer reconciliation between theory and experimental results can result. The creating photon may create particle vibration and spin as well as mass and linear motion. In pair production:

\[ h\omega_{v0} + (n + 1/2)h\omega_{s0} + (n + 1/2)h\omega_{m0} \]

In pair annihilation at least two photons must be produced which get their energy from the linear, vibrational and spin kinetic energies as well as the mass-energy conversion. \( h\omega_{v1} + h\omega_{s1} + h\omega_{m1} = 2mgc^2 + 1/2ma_0v^2 + 1/2ma_0v^2 + 1/2I\omega_{v0} + 1/2I\omega_{s0} + (n + 1/2)h\omega_{m0} \). While these experiments were performed with a BEC healing length, \( V_D \) happens twice per every period of the mirror oscillation at non-equivalent positions (hysteresis effect), which leads to a non-zero net energy loss. The cooling devices, which is based on the phenomenon of optical bistability. These devices are modeled as a Fabry-Perot resonator with one fixed and one oscillating mirror. Using a magnetically-tuned Feshbach resonance, the \( m_1 \) is reduced to zero near which \( \xi \) becomes very large. Results of applying the disorder potential to this nearly non-interacting condensate, with \( a_s \) much less than the Bohr radius, will be reported.

R1.00171 Compton Effect Energy Formulas Should Include Vibrational and Spin as well as Linear Kinetic Energies

STEWART BREKKE

Northeastern Illinois University (former grad student) — In Compton scattering the incident photon affects not only the linear, but also the vibrational and spin kinetic energies after impact. \( h\lambda_1 + m_0c^2 + 1/2ma_0v^2 + 1/2ma_0v^2 + (n + 1/2)h\lambda_1 = \frac{hc}{\lambda_1 + m_0c^2 + 1/2ma_0v^2 + 1/2ma_0v^2 + (n + 1/2)h\lambda_1} \). If the incident photon produces a relativistic speed, the equation should be \( h\lambda_1 + m_0c^2 + 1/2ma_0v^2 + 1/2ma_0v^2 + (n + 1/2)h\lambda_1 = \frac{hc}{\lambda_1 + m_0c^2 + 1/2ma_0v^2 + 1/2ma_0v^2 + (n + 1/2)h\lambda_1} \). By including the other kinetic energies a closer reconciliation between theory and experiment will occur.

1.\(^{1}\) previous papers presented at earlier APS meetings

R1.00172 Feedback-controlled radiation pressure cooling

YEHIAM PRIOR, MARK VILENSKY, ILYA SH. AVERBUKH, Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — We propose a new approach to laser cooling of micromechanical devices, which is based on the phenomenon of optical bistability. These devices are modeled as a Fabry-Perot resonator with one fixed and one oscillating mirror. The bistability may be induced by an external feedback loop. When excited by an external laser, the cavity field has two co-existing stable states depending on the position of the moving mirror. If the latter moves slow enough, the field in the cavity adjusts itself adiabatically to the mirror’s instantaneous position. The mirror experiences radiation pressure corresponding to the intensity value. A sharp transition between two values of the radiation pressure force happens twice per every period of the mirror oscillation at non-equivalent positions (hysteresis effect), which leads to a non-zero net energy loss. The cooling mechanism resembles Sisyphus cooling in which the cavity mode performs sudden transitions between two stable states. We provide a dynamical stability analysis of the coupled moving mirror – cavity field system, and find the parameters for efficient cooling. Direct numerical simulations show that a bistable cavity provides much more efficient cooling compared to the regular one.

R1.00173 Effect of Disorder on a Bose-Einstein Condensate with Tunable Interactions

D. DRIES, YONG P. CHEN, J. HITCHCOCK, M. JUNKER, T. A. CORCOVILLOS, C. WELFORD, R. G. HULET, Rice University Physics and Astronomy and Rice Quantum Institute — We have investigated the effect of a disordered optical potential on the transport and phase coherence of a Bose-Einstein condensate (BEC) of \(^6\)Li. We observe damping of BEC dipole oscillations even when the disorder strength, \( V_D \), is small, while for large \( V_D \), transport is completely inhibited. Time-of-flight images show that the BEC gradually loses phase coherence for \( V_D > \mu/2 \), with coherence completely lost when \( V_D = \mu \), where \( \mu \) is the chemical potential of the BEC. We interpret this loss of coherence as resulting from fragmentation of the BEC as seen from in-situ measurements of the density distribution. While these experiments were performed with a BEC healing length, \( \xi \), that is small in comparison to the disorder length scale, we are currently attempting to observe the Anderson localization predicted to occur for large \( \xi \). Using a magnetically-tuned Feshbach resonance, the s-wave scattering length, \( a_s \), is reduced to near zero where \( \xi \) becomes very large. Results of applying the disorder potential to this nearly non-interacting condensate, with \( a_s \) much less than the Bohr radius, will be reported.

1.\(^{\text{Supported by NSF, ONR, NASA, Welch}}\)

2.\(^{\text{Now at Purdue University}}\)

R1.00174 K-Shell Ionization of Atoms (2 \( \leq Z \leq 92 \))

M.A.R. PATOARY, Department of Physics, University of Rajshahi, Rajshahi, Bangladesh, M. ALFAZ UDDIN, Department of Physics, University of Rajshahi, Rajshahi, Bangladesh, A.K.F. HAQUE, Department of Physics, University of Rajshahi, Rajshahi, Bangladesh, A.K. BASAK, Department of Physics, University of Rajshahi, Rajshahi, Bangladesh, B.C. SAHA, Department of Physics, Florida A&M University, Florida-32307 — The electron impact ionization phenomenon have fundamental importance ranging from plasma to astro-physics. Reliable K-shell ionization cross sections (KICS) are needed for various quantitative analyses. Even the first order quantal calculations are rather both lengthy and not too easy to implement for various modeling calculations. We propose a parameter free model based on the widely used binary encounter approximation (BEA) [1,2] by incorporating both the ionic and relativistic corrections and have tested to evaluate KICS with considerable success as compared to experimental results even up to \( E = 1 \) GeV.


B.\(^{\text{CUS acknowledges the support from the NSF CREST}}\)

R1.00175 ARTIFICIALLY STRUCTURED MATERIALS –

R1.00176 Fabrication of metamaterials in THz region using ink jet system and characterization using THz-TDS

YEW LI HOR, HEE LIM, JOHN FEDERICI, NEW JERSEY INSTITUTE OF TECHNOLOGY TEAM — This article demonstrates the use of new fabrication techniques to fabricate metamaterials in THz range via a material deposition system. The patterns of these metamaterials follow the conventional designs which are single ring-SRR and double-Dots with varying conductivities. Highly conductive nano particle Ag and Pedot/PSS polymer inks are used as structural medium. The fabricated metamaterials of effective lattice sizes of 50 to 80 micron are then characterized using THz-TDS with 0.1 to 3 THz range in transmission mode. The detail steps of fabrication and THz-TDS experimental setup are elaborated. The absorption spectra of different thicknesses and different background substrate of these metamaterials are presented and discussed. Additional, the theoretical modeling of the fabricated samples are shown and compared with the experimental result.
A study of Diamond like Carbon films deposited by PECVD using DC and pulsed DC power supply.

R1.00187 Drift Instability of a 2D Magnetoplasma in a Periodic Potential. M. TAHIR, University of Sargodha, Sargodha, Pakistan, K. SABEEH, Quaid-i-Azam University, Islamabad, Pakistan, V. FESSATIDIS, Fordham University, Bronx, USA, N.J.M. HORING, Stevens Institute of Technology, Hoboken, USA — We examine the drift instability of a magnetized 2D electron plasma in a weak periodic potential, taking account of a steady current. In this, we treat a strong magnetic field inducing Landau quantization, and analyze both the inter- and intra-Landau band plasmon spectra within the framework of the random phase approximation, determining the occurrence of magnetoplasmon instability as a function of drift speed.

R1.00178 Stability and structure of free-standing III-V nanorods: An ab initio investigation. ROMAN LEITSMANN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller Universität Jena — The interest in anisotropic needlelike crystals has been recently stimulated by the potential need as building blocks for nanoscale electronic and photonic devices. Due to their considerable potential for optoelectronics or high-speed electronics nanorods (NRs) consisting of III-V semiconductors are of particular interest. In most cases the growth direction of III-V semiconductor NRs is parallel to the [111] axis of the bulk zinc-blende (zb) structure. However, the crystal structure of the NRs may change noticeably, depending on growth conditions and growth method. In particular, changes of the crystal symmetry from the cubic to the hexagonal (wurtzite - w) stacking of the carbon-anion bilayers have been observed in many cases. We report an investigation of hexagonal-shaped III-V III semiconductor NRs with varying crystal structure, varying surface passivation, and varying diameter [1]. Their stability is dominated by the free surface energies of the corresponding facets. We observe a phase transition between local zb and w geometry of the rods versus the preparation conditions of the surfaces [1] J. Appl. Phys. 102, 063528 (2007)

R1.00176 Bloch oscillation and Stark localization in graded lattices. KIN WAH YU, Chinese University of Hong Kong, K. YAKUBO, Hokkaido University, J. J. XIAO, Hong Kong University of Science and Technology — In this work, we report Bloch oscillation (BO) in graded elastic [1] and plasmonic [2] lattices. This is an unusual kind of oscillatory motion due to the band structure of graded lattices and is analogous to electronic BO in semiconductor superlattices. The study is related to the recently identified localized excitations called gradons which is peculiar to graded lattices [1,2]. We will use semiclassical theory to establish the conditions for BO and study the dynamics of BO in these systems. Moreover, we will confirm semiclassical solution by time-domain simulations of the propagation of wave packets. Results of these two methods will be compared. In this way, we can understand the origin of gradon localization more clearly. Results of the present research also offer great potential applications for controlling wave propagation by means of graded materials.

1Supported by RGC and JSPS

R1.00181 Modeling the self-assembly of nanoparticle and nanorod superlattices. ALEXEY TITOV, PETR KRAL, University of Illinois at Chicago, PROF. KRAL'S RESEARCH GROUP TEAM — Colloidl semiconductor PbSe/CdSE nanoparticles (NP) of the sizes of 3-10 nm can self-assemble in fcc, hcp and single-hexagonal (sh) superlattices [1]. We model the Coulombic, van der Waals and steric interactions between these NPs to understand the exact conditions under which they can self-assemble in these lattice structures. Our simulations show that non-local dipoles of the NPs and their screening by the conducting substrate are both crucial for the sh lattice formation. We model analogously the self-assembly of semiconducting CdSe nanorods (NRs), realized also in the presence of electric fields [2], and the binary semiconducting-metallic nanoparticle superlattices [3].


R1.00182 Experimental Study of Electrical Properties of ZnO Nanowire Random Networks for Gas Sensing and Electronic Devices. DAQING ZHANG, CSU Fresno, SIRISHA CHAVA, CHRIS BERVER, Univ. of Idaho, ANIRBAAN MUKHERJEE, VANVILAI KATKANANT, CSU Fresno — ZnO nanostructures are an attractive material for electronic and optical applications due to their many unique properties. Our research focuses on studying mats of ZnO nanowires as an electronic material with particular interest in their interaction with various gases. The ZnO nanowires were synthesized on sapphire substrates using a tube furnace at atmospheric pressure. Two-terminal current-voltage (I-V) measurements were used to examine the electrical conductivity of the ZnO nanowire mat as a function of temperature and exposure to various gases. The ZnO nanowires were synthesized on sapphire substrates using a tube furnace at atmospheric pressure. Two-terminal current-voltage (I-V) measurements were used to examine the electrical conductivity of the ZnO nanowire mat as a function of temperature and exposure to various gases. Temperature-dependent measurements were performed in vacuum using a continuous flow cryostat over ~150 K to ~ 300 K. Gas exposure experiments were conducted in a custom-built environmental chamber which was filled with various testing gases (Ar, CO, CO2, H2) at 30 bar or under vacuum. We observed reversible changes in the I-V characteristics as a function of gas exposure. For CO, the currents increased by a factor of about four. In addition, changes in the I-V behavior were found to be reversible after evacuation. Possible mechanisms for the gas-specific responses of the ZnO nanowire mat will be discussed.

R1.00183 CdSe, CdTe and core-shell CdSe-CdTe nanowires: A density functional study. R. RAMPRAASAD, TOM SADOWSKI, University of Connecticut — Semiconductor nanowires (NWs) are attractive in photovoltaic applications due to their ability to support a large number of electron-hole pairs (excitons) and the possibility of enhanced transport of dissociated charge carriers. To facilitate transport along the long axis of the nanowires, efficient charge separation of the exciton is desired. There is evidence suggesting that at a Type II band offset between two semiconductors enables charge separation more easily than in single component systems. The focus of this study is to provide an understanding of the tendency for electronic-hole separation in core-shell CdSe-CdTe NWs, which contain a radial Type II band offset. In particular, first principles computational methods have been applied to theoretically long CdSe-CdTe heterostructure NWs in the wurtzite crystal structure over a range of core and shell sizes. The interfacial energy of the nanorods, the band gaps, and the location of the electron and hole states are assessed as a function of the number of CdSe pairs, and core and shell radii. The overlap of the electron and hole wavefunctions, determined to quantify the extent of electron-hole separation, is differentiated with that for single-component CdSe and CdTe nanowires.
R1.00184 Fano effect in quantum wires with a uniform transverse electric field. V. VARGIAMLIS, Aristotle University, Thessaloniki, Greece, V. FESSATIDIS, Fordham University, Bronx, USA — We investigate the effect of an external uniform transverse electric field on the Fano resonance in electronic transport of a quantum wire with a finite range impurity. We employ the Feshbach coupled-channel theory for calculating the transmission probability. The attractive impurity is Pöschl-Teller along the propagation direction but is an arbitrary function of the lateral coordinate. For this type of impurity analytical solution to the scattering problem is possible. The Fano line shape resulting from the interference of direct transmission via a quasibound state created in the impurity, is shown to be strongly affected by the strength of the electric field. In particular, we show that as the strength of the electric field increases the resonance width continuously decreases and finally shrinks to zero. Consequently, the Fano line shape collapses. The vanishing of the resonance width indicates the transformation of the quasibound state into a true bound state in the continuum. Depending on the strength of the impurity, the collapse of the Fano line shape can even occur in the regime of weak electric field. This interesting collapsing behavior of the Fano resonance has also been shown to occur in purely one-dimensional systems (i.e., in 1D mesoscopic open rings). We also examine the role of the transmission amplitude, in the complex energy plane, as a function of the electric field strength.

R1.00185 Dynamics of an Electron in a Saddle Potential Subject to Crossed Electric and Magnetic Fields. K. SABEEH, A. YAR, Quaid-i-Azam University, Islamabad, Pakistan, V. FESSATIDIS, Fordham University, Bronx, USA, N.J.M. HOHLFELS, Stevens Institute of Technology, Hoboken, USA, M.L. GLASSER, Clarkson University, Potsdam, USA — We analyze the role of an electric field in the scattering/tunneling of an incident plane electron wave through a quantum point contact in a magnetic field. In this, the point contact is modeled as a saddle potential. We employ the Bogoliubov transformation and guiding center coordinates following the techniques of H. A. Fertig and B. I. Halperin (Phys. Rev. B 36, 7969 (1987)), but we expand the analysis to include the effects of the applied electric field here and examine the temporal development of the incident plane electron wave rather than that of a bath eigenfunction.

R1.00186 Magneto-optics of single Rashba spintronic quantum dots subjected to a perpendicular magnetic field. MANVIR KUSHWAHA, University of Puebla, Puebla, Mexico — We report on the theoretical investigation of the effect of the Rashba-type spin-orbit interaction (SOI) on the Fock-Darwin energy spectrum in the parabolically confined quantum dots in the presence of a perpendicular [to the original two-dimensional electron gas (2DEG)] magnetic field. The study is based on the exact analytical results obtained without any approximation and numerical simulation. We observe that the SOI modifies drastically the optical, thermodynamic, as well as magneto-optical properties of the (narrow-gap InAs) quantum dots. We discuss the dependence of the Fock-Darwin spectrum, Fermi energy, optical transitions, and magnetization on all the important parameters involved in the theory such as, for example, the orbital quantum number, the magnetic field, the confinement potential, and the Rashba parameter that characterizes the strength of the SOI. The illustrative examples include the results both with and without the SOI, for the sake of comparison. One of the most important observation is that the Rashba SOI causes the band mixing and band shifting in the quantum dots and the Fock-Darwin energy spectrum becomes richer but complex. This complexity seems to arise due to an intricate interplay between the SOI and the Zeeman energy.

R1.00187 Left-handed materials: detailed experimental parametric studies of the fishnet structure. V.D. LAM, J.B. KIM, J.W. PARK, N.T. TUNG, S.J. LEE, Y.P. LEE, q-Psi and BK21 Program Division of Advanced Research and Education in Physics, Hanyang University, Seoul, Korea — Recently, a new area of research, called left-handed materials (LHMs), has attracted considerable interests due to their unusual physical properties and novel applications. The first experimental evidence for the existence of LH behavior was proposed by Smith et al., using the right-handed resonator combined with the continuous wire. Several different designs, utilizing this idea for the LHMs, have been reported. Zhou et al. investigated the LHMs based on the H-shaped wires, which exhibits a negative refraction index in the microwave range. Dolling et al. introduced a modification with rectangular structures (the so-called fishnet structure) and demonstrated the LH characteristics at a wavelength of 780 nm while S. Zhang et al. employed an array of elliptical apertures, showing the LH behavior in the near-infrared regime. The main purpose of these modified structures is to find out the optimized structure that can be easily fabricated and experimentally characterized, especially, LHM working at optical frequencies. In this report, we present the experimental results of the parametric study on the fishnet structure, which are also compared with the previous theoretical studies. These structures were designed, fabricated, and measured in the microwave frequency regime.

R1.00188 Nonlinear Fano effect in semiconductor quantum dots: Detecting weak interactions. ALEXANDER GOVOROV, Ohio University — The Fano interference effect appears when a discrete state of an atom or quantum dot couples with a continuum of states. In self-assembled quantum dots, the coupling may come from the tunnelling or Auger processes [1,2,3]. This study develops a theory of Fano effect in self-organized quantum dots under the condition of strong optical pumping. Our theory shows that the Fano effect becomes greatly enhanced in the nonlinear regime. In the linear regime, if the dot-continuum interaction is very weak, the optical detection of Fano effect is impossible because of the Heisenberg principle. In other words, in the linear regime, a finite lifetime of an exciton creates an energy uncertainty and the Fano interference effect becomes invisible. However, in the nonlinear regime, the natural radiative broadening does not play the main role and even a very weak dot-continuum interaction becomes apparent. This nonlinear method can be used to detect very weak interactions between a two-level system (or qu-bit) and a continuum of states of any nature. The nonlinear Fano effect in InAs quantum dots has been observed in the recent experiments performed in Munich and Edinburgh [3]. This study was performed in collaboration with W. Zhang, R. J. Warburton, K. Karrai, and R. J. Warburton. [1] A.O. Govorov, R. J. Warburton, and K. Karrai, Phys. Rev. B 67, 241307 (2003). [2] K. Karrai et al., Nature 427, 135 (2004). [3] M. Kroner et al., submitted to Nature.

R1.00189 Optically Injected Charge and Spin Density Patterns in Quantum Wells1. JOHN SIPE, RASHAD ABRAROV, EUGENE SHERMAN, Department of Physics and Institute of Optical Sciences, University of Toronto — We investigate the charge and spin dynamics following optical injection of currents in quantum wells taking into account momentum relaxation, electron-hole drag and the long-range Coulomb forces. Our numerical approach uses expansion of the investigated quantities in the Hermite-Gaussian basis. We find that on time scale of the order of one nanosecond the carrier and current densities demonstrate complex patterns even when the effects of the spatially nonuniform forces are expected to be weak. This behavior can be attributed to two different processes: the charge displacements seen in the THz radiation and optical pump-probe experiments can be sufficiently different. The resulting spin density patterns arising due to the spin-dependent electron-hole skew scattering are calculated and analyzed in terms of the spin-orbit coupling, Coulomb forces, and the carrier momentum relaxation effects.

1We are grateful to the NSERC (Canada) for support.

R1.00190 Computational Study on the Magneto-optical Effects from Gyrotropic Gratings. MIN HYUNG CHO, YUE HUI LU, Y. P. LEE, Quantum Photonic Science Research Center, Hanyang University, Seoul, Korea, J00 YULL RHEE, BK21 Program Division of Advanced Research and Education in Physics Research Division and Institute of Basic Sciences, Sungkyunkwan University, Suwon, Korea — Maxwell’s equations with non-diagonal complex dielectric tensor are numerically studied for the calculation of Magneto-optical(MO) effects from one-dimensional lossy gyrotropic or magnetic gratings. Owing to the periodicity of the structure, the dielectric tensor is expanded out in Fourier series and the electric and the magnetic vectors are written in terms of Bloch wave. Then, Maxwell’s equations are simplified as a system of ordinary differential equations, and the solutions can be simply written in terms of exponential function with the eigenvalue of system times the initial value. Finally, by considering the multiple reflection in the grating structure with Airy-like internal reflection series, the reflection and the transmission matrices are obtained and used to calculate the MO effect. The Kerr rotations of the 0th and the 1st diffracted orders are calculated as a function of various parameters. The calculated results agree excellently with the experimental data for permalloy gratings. This method can also be used for many interesting applications and easily extended to two-dimensional gratings.
Giant Photonic Band Gaps in one dimensional Photonic heterostructures. In this work we show that it is possible to design Giant Photonic Band Gaps in heterostructures via the determination of the group velocity. A photonic heterostructure is composed by the union of two or more distinct photonic crystals. We present the calculation of the heterostructure band structure implementing the supercell technique in the plane wave method. We show that even if the heterostructure presents a very complicated photonic band structure, it is possible to discriminate the regions of low transmission obtaining the group velocity. We verify the very existence of the forbidden allowed regions with the theoretical calculations of the light transmission.

Two-dimensional photonic crystal heterostructure with Omnidirectional band gap. We present the numerical determination of giant omnidirectional (3D) photonic band gaps calculated for a two-dimensional heterostructure, which are composed by the union of two photonic crystals. The photonic band structure is calculated via the implementation of the supercell technique on the the plane-wave method. We have optimized the structure in order to obtain the biggest band gap.

Synthesis and study of composite silver-polymer metamaterials. We have designed, synthesized and characterized a range of non-magnetic metamaterials with continuously tunable dielectric constant. Powders of 30 nm silver nanoparticles were suspended onto glass substrates and characterized in optical transmission and reflection experiments. Using known formula for reflectivity and transmissivity in three-layered structures, we extracted from the experimental data the spectra of real and imaginary parts of the effective dielectric constants. The experimental maximal value of $\varepsilon_{eff}'$ exhibited monotonous growth and reached $\varepsilon_{eff}'=12.8$ at $\lambda=2.4 \mu m$ at the maximal concentration of Ag nanoparticles. The demonstrated value of $\varepsilon_{eff}'$ exceeds that in Si and appears to be the highest in 1.5-2.5 $\mu m$ spectral range. The demonstrated easy-to-synthesize nanoparticle adds to the tool box of photonic metamaterials with extreme values of $\varepsilon$.

Magnetic dipole systems for probing optical magnetism. Powders of 30 nm silver nanoparticles were suspended in solution of Polymethylmethacrylate and exposed to Q-switched laser radiation in order to separate nanoparticles and/or reduce the degree of aggregation. The films of Ag-PMMA composites were deposited onto glass substrates and characterized in optical transmission and reflection experiments. Using known formula for reflectivity and transmissivity in three-layered structures, we extracted from the experimental data the spectra of real and imaginary parts of the effective dielectric constants. The experimental maximal value of $\varepsilon_{eff}'$ exhibited monotonous growth and reached $\varepsilon_{eff}'=12.8$ at $\lambda=2.4 \mu m$ at the maximal concentration of Ag nanoparticles. The demonstrated value of $\varepsilon_{eff}'$ exceeds that in Si and appears to be the highest in 1.5-2.5 $\mu m$ spectral range. The demonstrated easy-to-synthesize nanoparticle adds to the tool box of photonic metamaterials with extreme values of $\varepsilon$.

Artificial Molecules. Confinement of carriers in quantum dots results in hydrogenic like states for the exciton. Thus a single excitation in a quantum dot bears resemblance to a hydrogen atom; these materials are often referred to as ‘artificial atoms’. A pair of excitons will form a four body biexciton, akin to a hydrogen molecule. Quantum confinement increases the binding energy of the ground state of the biexciton. Quantum confinement should also produce bound states for the excited states of the biexciton. Thus the excitonic ‘hydrogen molecule’ should have an eigenstate spectrum in the vein of molecular orbitals. The eigenstate spectrum of the biexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of excited states of the biexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems.

Hollow Quantum Dot Shells: Optical Response Function Analysis. We consider the response of finite two-dimensional lattice shells of coupled quantum dots, approximated as dipoles, to an applied external electric field. We assume that the lattice constant is much smaller than the wavelength of applied electric field, to provide a coherent exciton. Using the matrix Green's function and Coupled Dipole Hamiltonian, the response function is derived and analyzed numerically. Treating the dipole coupling as a parameter, the response function of an entirely decoupled lattice is calculated, from which the coherence effects are determined in the fully coupled case. The effect of hollowness is considered, in which optical resonator effects are determined, resulting from the matching of the radius of the cylindrical shell to the light wavelength. The response function is decomposed into partial response functions due to individual modes, in which the polarization dependence is determined by altering the orientation of the incident field.

Wave Transmission Through a Nano-hole. We have examined the integral equation for scalar wave transmission through a nano-hole modeled as a single point, employing a formal procedure for an exact analysis. The dependence is determined by altering the orientation of the incident field. The response function is decomposed into partial response functions due to individual modes, in which the polarization dependence is determined by altering the orientation of the incident field.

Nanostructured Silicon Optical Waveguides. We have measured the group index in both the TE and TM polarizations, and the experimental values agree closely with computational simulations using a fully-vectorial finite-difference mode-solver. We have fabricated and demonstrated multi-slot waveguides in silicon-on-insulator chips, with slot width 100 nm and slot-to-slot spacing of 150 nm. For chip-scale optical delay lines and compact waveguide-based polarization switches incorporating phase retardation. Using electron-beam lithography and dry etching, we have fabricated and demonstrated multi-slot waveguides in silicon-on-insulator chips, with slot width 100 nm and slot-to-slot spacing of 150 nm.

This work was supported by CONACYT 60897 project.
R1.00199 Förster Resonance Energy Transfer between Nanoparticles and Nanowires . PEDRO L. HERNANDEZ-MARTINEZ, ALEXANDER O. GOVOROV, Ohio University — We develop a theoretical model to describe Förster resonance energy transfer (FRET) between semiconductor nanoparticles (NPs) and nanowires (NWs). We obtain an analytical equation in the dipole limit and a numerical solution for the general case. We find that, for FRET between NPs and NW, the transfer time is proportional to 1/d^5, where d is the distance between NP and NW. The calculated transfer time between CdTe NPs and NWs is 16.9 ns. This number agrees well with the experimental value, 16 ns [1]. We also found good agreement with the experimental data [1] for other NP-NW distances. For a NW material, we explore a semiconductor (CdTe) and metals (Au and Ag) [2]. In a NP-NW bio-conjugate, excitons flow from NPs to a NW and then become collected in the NW. When voltage is applied across a NW, this system is expected to demonstrate enhanced photo-current and photo-voltage responses. The enhancement effect comes from energy channeling from NPs to a NW due to FRET. This system can be used in optoelectronic devices and energy conversion systems. [1] J. Lee, A. O. Govorov, and N. A. Kotov, Nano Letters 5, 2063-2069 (2005). [2] J. Lee, P. Hernandez, J. Lee, A. O. Govorov, and N. A. Kotov, Nature Materials, 6, 291 – 295 (2007).

R1.00200 Nanometer sized electrodes fabricated by electromigration of Au and Pd nanowires . ALEXANDRU VLAD, SÉBASTIEN FANIEL, BENOIT HACKENS, VINCENT BAYOT, SORIN MELINTE, DICE - Université Catholique de Louvain, Louvain la Neuve, Belgium — Electromigration-driven metallic nanowire failure is presented. Here, Au and Pd nanowires patterned by electron-beam lithography were electrically stressed up to their breaking point. Feedback control and simple voltage sweep techniques have been successfully used to form nanometer-sized gaps. We observe a decrease in residual resistance up to the breaking point. In contrast, Pd nanowires presented an anomalous resistance decrease close to their failure point. This was associated to the melting and agglomeration of metallic grains within the electrically stressed nanowires. The SEM images acquired at intermediate stages of electromigration agree with the electrical data findings. The influence of the nanowire geometry upon the morphology of fabricated nanoelectrodes is considered. Beside the morphological characterization of our break junctions, we also measured their current-voltage characteristics. We observed single electron tunneling effects, probably due to the presence of metallic clusters formed close to the nanoelectrodes during the electromigration. Our results are consistent with recent findings on Coulomb blockade phenomena in electromigrated gold break junctions.

R1.00201 Molecular spin clusters for quantum computation . MARCO AFFRONTE, CNR-INFM-S3 — Molecular spin clusters are prototypical systems exhibiting coherent dynamics of the electronic spin. The pattern of the lowest lying spin states is well defined and controlled at the synthetic level. The chemical bottom up approach used for the synthesis of molecules also allows to reduce intrinsic sources of decoherence and to build links between clusters, thus creating entanglement of spin states. Molecular spin clusters can be deposited at surfaces, thus forming scalable networks. Different molecules and ligands may be combined to exploit different functionalities, the latter being defined at molecular level. These facts provide extraordinary motivation to attempt the implementation of molecular quantum processors that, in turn, are test bench for novel quantum algorithms. Recent achievements obtained on antiferromagnetic molecular rings will be presented.

R1.00202 Quantum Computing using Rotational Modes of Dimers . KENJI MISHIMA, KOICHI YAMASHITA, Univ. of Tokyo — In this paper, we numerically constructed general-purpose phase-correct global quantum gates by using intermolecular rotational modes of two polar molecules coupled by dipole-dipole interaction to encode two qubits and implement the Deutsch-Jozsa algorithm. The calculations were based on the multi-target optimal control theory (MTOCT). The molecular systems we examined were NaCl-NaBr, NaCl-NaCl, and NaBr-NaBr dimer systems. The rotational states in the ground vibrational state of the ground electronic state of these pairs were taken as two qubits. When implementing the Deutsch-Jozsa algorithm by combining these elementary gates, we obtained a maximum probability 97.95 % for NaBr-NaBr system with the interval R=5.0 nm in the repulsive configuration, which is the best performance of the two-state Deutsch-Jozsa algorithm compared with intramolecular vibrational-vibrational, rotational-vibrational, and electronic-vibrational qubits reported so far.

R1.00203 Thermal conductivity of Si nanocrystals1 . SHANG-FEN REN, Illinois State University, WEI CHENG, Beijing Normal University — Thermal conductivities of spherical Si nanocrystals (NCs) are investigated with three different models: a macroscopic approximation, a semi-microscopic model that calculates the heat capacity of NCs with a microscopic Valence-Force-Field Model (VFFM), and a full microscopic description of phonon thermal conduction that calculate both heat capacity and phonon group velocity by the VFFM. The results are compared, and the advantages and limitations of each of these models are discussed. It is shown that for spherical Si NCs, the macroscopic approximation is quite good for NCs with a diameter larger than 1.33 nm. For smaller NCs, the VFFM predicts that the thermal conductivity increases quickly when the size decreases, opposite to the macroscopic approximation, and VFFM also predicts that the minimum of thermal conductivity for spherical Si NCs occurs at a diameter of 1.33 nm, the limit at which the macroscopic approximation applies.

1SFR acknowledges the support by Research Corporation (CC6274)

R1.00204 Thermoelectricity in Ca$_3$Co$_4$O$_9$: An Atomic Structure Perspective1 , T. TYSON, Z. CHEN, New Jersey Institute of Technology, J. TU, City College of New York, Q. LI, Brookhaven National Laboratory — The temperature dependent local structure about the Co sites in the misfit system referred to as Ca$_3$Co$_4$O$_9$ was examined by x-ray absorption spectroscopy. Density Functional calculations utilizing a large cell were used to obtain the optimized atomic structure. The detailed atomic structure about the Co sites was determined from the XAFS measurements. The complementary density functional computations of the structure and atomic forces provide a new 3D model of the structure and point to a unique configuration which may be the origin of the high thermoelectricity in this material.

1This research was funded by NSF DMR-0512196.

R1.00205 Maximizing thermoelectric figure-of-merit at high temperature in p-type Bi-Sb-Te system . BO YU, YI MA, JIAN YANG, BED POUDEL, YUCHENG LAN, DEZHI WANG, ZHIFENG REN, Dept. of Physics, Boston College, QING HAO, GANG CHEN, Dept. of Mechanical Engineering, Massachusetts Institute of Technology, DEPT. OF PHYSICS, BOSTON COLLEGE COLLABORATION, DEPT. OF MECHANICAL ENGINEERING, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION — Bismuth telluride alloys and their derivatives are the most important thermoelectric materials used in refrigeration devices around room temperature. Using mechanical alloying and hot press, we have achieved 100% dense nano-structured p-type Bi$_3$Sb$_2$Te$_3$ samples. We demonstrated here that the enhanced dimensionless figure-of-merit (ZT) are due to enhanced phonon-scattering, and the ZT peak could be easily shifted to higher temperature by varying the composition and processing conditions.

R1.00206 Thermoelectric Properties Studies on n-type Bi$_2$Te$_3-x$Se$_x$ . JIAN YANG, XIAO YAN, YI MA, BED POUDEL, YUCHENG LAN, D.Z. WANG, Z.F. REN, Physics Department, Boston College, Chestnut Hill, MA02467, Q. HAO, G. CHEN, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — Bi$_2$Te$_3-x$Se$_x$ is a classic room temperature n-type thermoelectric material. In spite of the long history of research, its ZT is still below 1. By directly making nano sized particles using mechanical alloy from element, then pressing the nanoparticles into 100% dense bulk sample with nano-structures by hot press, we expect to decrease the thermal conductivity by the increased grain boundary scattering of phonons so to improve the ZT above 1. The ratio of Te/Se was varied systematically to investigate its effect on thermal conductivity.
R1.00207 Thermionic cooling on barium strontium thin film surface\(^1\), FENG JIN, GUOGANG QIAN, SCOTT LITTLE, Ball State University — Strong thermionic emission was observed from low-work-function barium strontium oxide thin films. Such strong thermionic emission resulted from a cooling effect on the emitting surface. Temperature drops as high as 90 °C were obtained. Barium strontium oxide (BaSr\(_2\)O) thin films approximately 1 \(\mu\)m in thickness were deposited on tungsten substrates using RF magnetron sputter deposition. Thermionic emission from the thin film was characterized and the work function of the thin film was measured using Richardson line method. The temperature drop or cooling of the thin film surface at different emission current was measured using a high precision optical pyrometer.

\(^1\)This work was supported by the Department of Energy under contract No. DE-FC26-04NT42329.

R1.00208 Mn linear chains deposited on CuN/Cu(001): environment effects on the Mn-Mn interactions, MARIA ANDREA BARRAL, Departamento de Física, FCEyN, Universidad de Buenos Aires, ANA MARIA LLOIS, Departamento de Física, FCEyN, Universidad de Buenos Aires, RUBEN WEHT, Departamento de Física, CNEA, GUSTAVO LOZANO, Departamento de Física, FCEyN, Universidad de Buenos Aires — Scanning tunneling microscopy (STM) was used recently to study the interaction among manganese atoms deposited on thin insulating copper nitride islands grown on Cu(001). The value of the exchange interaction \(J\) among manganese atoms for different atomic arrangements was obtained, showing that it strongly depends on the Mn deposition sites. In this contribution we present the result of ab initio calculations for different arrangements of infinite Mn chains on CuN/Cu(001) to understand the influence of the environment on the Mn-Mn exchange interactions.

R1.00209 Photopatterning in phase separating reactive ternary systems, PRATYUSH DAYAL, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — We investigate a ternary ABC phase separating system in which components A and B undergo reversible photochemical inter-conversion reaction while component C remains non-reactive. We focus on systems with unequal forward and backward reaction rates. It has been well known that in such binary systems the competition between phase separation and chemical reaction results in hexagonal patterns contrary to lamellar structures for equal reaction rates. Since the chemical reaction favors miscibility a phase diagram is established to determine the phase boundary of such systems. We demonstrate that by confining chemical reaction to designated places using masks more complicated structures could be formed in the binary AB systems. We elucidate the scenarios in which the third non-reactive C component results in the displacement of AB domains from the reaction sites in favor of C. This migration is driven by difference in the free energies between the reaction sites and the masked regions. A rich variety of complex super-lattice patterns can be formed by changing the processing variables such as initial concentration, distance between the masks and rates of forward and backward reaction.

R1.00210 Self assembled silicon nanowire Schottky junction assisted by collagen\(^1\), DIDIER STIEVENARD, IEMN - DptISEN, BILLLE SAHIL, IEMN-Dpt ISEN, YANNICK COFFINIER, RABAH BOUKHERROUB, IRI FRE2963, OLEG MELNYK, IBL UMR8525, IEMN - DPTISEN TEAM, IRI TEAM, IBL TEAM — We present results on self assembled silicon nanowire Schottky junction assisted by collagen fibrous. The collagen is the principle protein of connective human tissues. It presents the double interest to be a low cost biological material with the possibility to be combed as the DNA molecule. First, the collagen was combed on OTS modified surface with gold electrodes. Second, silicon nanowires were grown on silicon substrate by CVD of silane gas (SiH\(_4\)) at high temperature (500 °C) using a vapor-liquid-solid (VLS) process and gold particles as catalysts. In order to increase electrostatic interaction between the collagen and the nanowires, these latters were chemically modified by mercaptopropylmethoxysilane (MTPS), then chemically oxidized. Therefore, the nanowires were transferred from their substrate into water and a drop of it deposited on the surface. Nanowires are only bound to collagen and in particular, in electrode gaps. The formation of spontaneous Schottky junction is demonstrated by current-voltage characteristics.

\(^1\)This work was supported by DGA, under contract REI 0534048.

R1.00211 COMPUTATIONAL METHODS: DYNAMICS, TRANSFER, AND PLASMA —

R1.00212 Merging for Complex Particle Kinetic modeling of multiple plasma beams (inter-penetrating flows)\(^1\), ALEXANDER LIPATOV, GEST Center UMBC — We suggest a merging procedure for the Complex Particle Kinetic (CPK) model in case of inter-penetrating flow (multiple plasma beams). Each CPK macro-particle includes a Maxwellian distribution in velocity and Gaussian distribution in space with internal dynamics (see [Hewett, 2003], for details). It is assumed that an arbitrary distribution of real particles can be represented by such a superposition in phase space (moving—finite—element approach) at least as well as could be done with the standard particle in cell (PIC)/Monte Carlo (MC) delta functions and their associated “shape factors”. The CPK method allows us to provide a global simulation of the complex plasma objects on the Hall-MHD (fluid) scale (aggressive merging) with automatic incorporation of the kinetic/particle description of the particle-wave processes (aggressive fragmentation) where it is necessary. The CPK approximation works well for ions, electrons, dust grains and neutral components. This code was tested in the simulations for the study of the interaction of the plasma flow with comets and Io’s atmosphere. In this report we examine the standard (PIC) and the CPK methods in the case of the particle acceleration by shock surfing. The plasma dynamics is described by a standard (particle-ion– fluid- electron) hybrid model. While a particle-mesh study of the interaction of the plasma flow with comets and Io’s atmosphere is required to understand the high radiative power losses associated with tungsten. The energy loss due to radiative processes for high-Z ions can be critical in understanding the ionization balance of the plasma. We present non-local thermodynamic equilibrium (non-LTE) calculations for a tungsten plasma using the Los Alamos National Laboratory suite of atomic codes. We examine the radiated power losses and ion balance distributions for a variety of electron temperatures ranging from 2 keV to 30 keV and densities associated with conditions found in ITER.

\(^1\)This work was supported by the Department of Energy through Los Alamos National Laboratory.
or minor grooves. Differences between complexation with PEI and PLL will be discussed. The DNA does not undergo any major structural changes upon complexation and remains in the B-form. In the formed gene therapy vectors, with polycations emerging as promising candidates. Molecular dynamics simulations of the DNA duplex CGCGAATTCGCG in the presence to provide insight into the structure and formation of DNA polyplexes. After an initial separation of approximately 50 Å, the DNA and polycation come together to form a stable complex within 10 ns. The DNA does not undergo any major structural changes upon complexation and remains in the B-form. In the formed complex, the charged amine groups of the polycation mainly interact with DNA phosphate groups, and rarely occupy electronegative sites in either the major or minor grooves. Differences between complexation with PEI and PLL will be discussed.
Co-operative Macromolecular Disassembly via the Heat Shock Chaperone Hsc70. JASON PUCHALLA, KELLY KRANTZ, ROBERT AUSTIN, HAYS RYE, Princeton University — Many essential cellular functions depend on the assembly and disassembly of macromolecular complexes. A general class of protein known as molecular chaperones regulates several of these processes. How can complex protein structure be quickly and efficiently disassembled by the action of a small number of these proteins? One such example is that of clathrin: a ubiquitous protein that stabilizes vesicular trafficking by forming a scaffold onto the membrane surface. This scaffold must be removed before the vesicle can deliver its cargo. We report on the cooperative disassembly of yeast-derived GFP-labeled clathrin baskets via its interaction with Hsc70. We exploit the highest signal-to-noise light bursts from single fluorescent baskets transiting a confocal excitation spot to reversibly determine the brightness and size distribution of the baskets during the uncoating process. This minimal uncoating system demonstrates the ability of a surprisingly simple protein system to facilitate rapid structural changes through cooperative action.

3Supported by NIH (GM065421), NSF (DMR-0213706) & NJCSCR (06A-004-SCR3).
R1.00229 Linking Inverse Square Law with Quantum Mechanical Probabilities, SHANTILAL GORADIA, Gravity Research Institute, Inc. — (©2007 by S Goradia) I modify the Newtonian inverse square law with a postulate that the probability of interaction between two elementary particles varies inversely as the statistical number of Planck lengths separating them. For two nucleons a million Planck lengths apart, the probability of an interaction is a trillionth (almost never), seemingly contradicting gravity. Likewise, statistical expression of the size of the universe implicitly addresses the issue of dark energy by linking fine-structure constant \( \alpha = 1/137 \) with the cosmological constant \( \lambda = 1/R^2 \) (abstract submitted 11/11/07 for APS APR2008 meeting). Since light travels one Planck length per Planck time, the radius \( R \) of the spherical shape of the universe is \( 10^{60} \) Planck lengths, linking the cosmological constant \( \lambda = 1/10^{120} \) (see equation 14 in Einstein’s 1917 paper) with \( \alpha \) by the relationship \( 1/\alpha \approx \ln(1/\lambda) \). Intuitive answers to the questions raised suggest that the elementary particles interact via Planck scale mouths \(^1\) with higher probabilities at smaller distances. This intuition may be supported by genetics, explaining issues such as DNA – nucleosome interaction \(^2\)(3). \[1\] http://www.arxiv.org/pdf/physics/0211040 [v. 3] \[2\] www.gravityresearchinstitute.org \[3\] Segal E. et al, A genomic code for nucleosome positioning. Nature 442, pp. 772-778, 2006.

R1.00230 Fullerenes Can Induce Toxic Physical Changes of DNA, FABIAN C泽REWSKI, LENE B. ODDER-SHEDE, Niels Bohr Institute, Copenhagen, Denmark — Fullerenes are fascinating symmetric carbon nanostructures. Nowadays, they are widely used because of their characteristic physical and chemical properties. Until now research has mainly been focused on commercial applications of fullerenes. Only a few investigations have addressed the potential biological hazards, one of which is that fullerenes are believed to alter the elastic properties of DNA upon binding. In our experiments we use optical tweezers with sub-picoNewton and nanometer resolution to probe the structural changes and the potential damages which fullerenes might induce on single DNA molecules. Therefore, force-extension relations can be obtained under physiological conditions while varying the concentration of different types of fullerenes. It has theoretically been predicted \(^1\), that certain fullerenes can function as a minor-groove binder to double-strand DNA, thus altering its elastic properties significantly. Fullerenes are capable of causing severe damage inside living organisms by forming DNA regions which are not accessible for proper enzymatic functions. A further goal of the study is to establish fullerenes as a tool for a more detailed investigation of DNA-protein interactions, such as the trafficking of polymers or the packing by procaryotic proteins. \[1\] Zhao X, Striolo A, and Cummings PT: C60 Binds to and Deforms Nucleotides. BiophysJ (89):3856-62, 2005.

R1.00231 A study of the stability of the DNA double helix in complexes of DNA with the bipyridyl-(ethylenediamine)platinum(II) molecular ion, ATTILA SZABO, SCOTT LEE, University of Toledo — The DNA double helix is usually stabilized by the formation of a complex with a ligand. However, the exact nature of the complex can destabilize the double helix, as is well known in complexes of DNA with diaminedichloroplatinum(II). We report the results of our study of the complex of DNA with bipyridyl-(ethylenediamine)platinum(II), abbreviated [(bipy)Pt(en)]\(^2+\), via ultraviolet melting experiments. We find that the DNA double helix is stabilized by the formation of the complex: the temperature of the onset of melting of the DNA double helix increases with increasing amounts of [(bipy)Pt(en)]\(^2+\). The onset temperature is increased by about 14 °C for a ligand content of one [(bipy)Pt(en)]\(^2+\) for every three DNA base pairs.

R1.00232 From frontier states to an inter-nucleotide potential for DNA: a density functional theory based study, MARIA FYTA, Department of Physics, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — We present results from accurate density functional theory based simulations of individual DNA bases and representative base-pairs in various relative configurations, as they are likely to appear in the equilibrium and stretched forms of DNA. Specifically, we extract the salient features of electronic structure of these molecules, and reveal that the frontier states in the base pairs are related to only one component of the pair. For all combinations of bases and base pairs studied here, the nature of these states was not affected by separation of the bases or base pairs along different directions or rotation along the helical axis. From the same calculations we were able to parametrize and construct an optimized intermolecular potential for DNA nucleotides, that accounts for hydrogen bonding, stacking interactions and the contribution from the sugar backbone. These calculations serve to set the stage for more extensive coarse grain calculations of DNA related biophysical phenomena.

R1.00233 Drug-Membrane Interactions Studied by Vibrational Sum-Frequency Spectroscopy , LAUREN WOLF, KIMBERLY BRIGGMAN, NIST — The activity of a number of drugs depends directly on their interaction with cell membranes and, thus, an understanding of drug-membrane interactions is necessary for improving their pharmacological performance. Drug molecules can interact with membranes by directly binding to membrane-bound proteins or by intercalating into the lipid matrix itself, altering membrane properties such as fluidity, thickness, internal pressure, and phase transition temperature. Here, we focus on the effects of local anesthetics incorporated into the lipid matrix, studying the structural changes induced in supported lipid bilayers by vibrational sum-frequency spectroscopy (VSFS). We find that in addition to depressing the phase transition temperature of the lipid bilayers, most anesthetics also sharpen the gel to liquid-crystalline transition, suggesting an increase in membrane constituent cooperativity. This behavior contrasts the effects of cholesterol on lipid bilayers, which increases membrane rigidity and broadens the phase transition. The structure of the membrane-intercalated anesthetics themselves will also be discussed. This work demonstrates the potential of using supported lipid bilayers and surface-sensitive techniques for future pharmacological studies.

R1.00234 Structure of Functional Staphylococcus aureus \( \alpha \)-Hemolysin Channels in Tethered Bilayer Lipid Membranes, FRANK HEINRICH\(^1\), Carnegie Mellon University, GINTARAS VALNICUS, Institute of Biochemistry, Vilnius, DUNCAN J. MCGILLIVRAY\(^2\), Carnegie Mellon University, JOSEPH W.F. ROBERTSON, NIST Electronics and Electrical Engineering Lab., ILJA IGNATJEV, Institute of Biochemistry, Vilnius, JOHN J. KASIANOWICZ, NIST Electronics and Electrical Engineering Lab., MATHIAS LOESCHE\(^3\), Carnegie Mellon University — We demonstrate the functional reconstitution of the Staphylococcus aureus \( \alpha \)-hemolysin channel in membranes tethered to gold. Electrical impedance spectroscopy measurements show that the pores have essentially the same properties as those formed in free-standing bilayer lipid membranes. Neutron reflectometry (NR) provides high-resolution structural information on the interaction between the channel and the disordered membrane, and validates predictions based on the channel x-ray crystal structure. NR also shows that the proximity of the solid interface does not affect the molecular architecture of the protein-membrane complex. The results suggest that this technique could be used to elucidate molecular details about the association of other proteins with membranes. It also may provide structural information on domain organization and stimulı-responsive reorganization for transmembrane proteins in membrane mimics.

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R1.00235 Molecular Dynamics Simulated Annealing Study of Gramicidin A in Water and the Hydrophobic Environment. TAKAHARU MORI, YUKO OKAMOTO, Department of Physics, School of Science, Nagoya University and JST-BIRD — Gramicidin A is a hydrophobic 15-residue peptide with alternating D- and L-amino acids, and it forms various conformations depending on its environment. For example, gramicidin A adopts a random coil or helical conformations, such as \( \beta^{4.1}\text{-helix, } \beta^{6.3}\text{-helix, and double-stranded } \beta\text{-helix in organic solvents. To investigate the structural and dynamical properties of gramicidin A in water and the hydrophobic environment, we performed molecular dynamics simulated annealing simulations with implicit solvent based on a generalized Born model. From the simulations, it was found that gramicidin A has a strong tendency to form a random-coil structure in water, while in the hydrophobic environment it becomes compact and can fold into right- and left-handed conformations of \( \beta\text{-helix structures. We discuss the folding mechanism of the } \beta\text{-helix conformation of gramicidin A.} \)

R1.00236 Photo- and bio-physical characterization of novel blue and near-infrared lipophilic fluorophores for neuronal tracing. JEFF TONNIGES, MARIA HANSEN, Creighton University, Department of Physics, BERND FRITZSCH, Creighton University, Department of Biomedical Sciences, BRIAN GRAY, Molecular Targeting Technologies Inc., MICHAEL NICHOLS, Creighton University, Department of Physics. Lipophilic fluorescent dyes have been used to track neuronal connections because of their ability to diffuse laterally between nerve cell membranes. Given the large number of connections that a typical neuron makes with its neighbors, a diffusion-matched set of spectrally distinct dyes is desirable. Previously, a trio of dyes was developed with well-separated green, red and far red fluorescence emission that permitted triple labeling [1]. To extend this set to five, we have been characterizing the properties of novel blue and near-infrared candidates. By combining two-photon and confocal microscopy all of these candidates can be imaged using a single Ti:S laser. Here we present measurements of the absolute two-photon excitation spectra along with single- and two-photon fluorescence recovery after photobleaching measurements of the diffusion coefficient in spinal cord samples. [1] H. Jensen-Smith et al., Immunol. Invest., in press, 2007.

R1.00237 Coupled Translational and Rotational Fluctuations of Tethered Beads. ANDREW SPAKOWITZ, SHAFIGH MEHRAEEN, Stanford University — Single-molecule manipulation plays an important role in determining the physical mechanisms responsible for biological function. Establishing a robust method of predicting the fluctuating behavior of a tethered bead provides insight into how to maximize the signal-to-noise ratio to improve experimental resolution. We theoretically address the behavior of single-molecule experimental apparatuses. Our theory is amenable to addressing a variety of different bead-tether systems, thus providing a basis for comparing and contrasting these different experimental setups and for adapting the theory to the specific experimental system of interest. Fluctuations in both the location and orientation of the bead are incorporated in the theory; we explore their coupled effect on the observed behavior in single-molecule systems. The physical behavior of the tether molecule is described using the wormlike chain model. Making use of our exact solutions for wormlike chain model statistics, our current treatment achieves exact precision for the polymer behavior, apart from the approximations that are inherent to the wormlike chain model. We find that the impact of rotational fluctuations on the bead motion is largest when the radius of the bead is comparable to the length of the chain tether. We explore the impact that chain length and bead radius have on the resolution of single-molecule experiments and how to maximize the signal-to-noise ratio.

R1.00238 Formation of highly ordered self assembled monolayers of alkanethiol molecules on thermally annealed gold films. YOUNG-KYU HONG, HYUNYUNG YU, TAE GEOL LEE, NOAH LEE, JAE HO BAHNG, NAM WOONG SONG, WON CHEGAL, HYUN KYONG SHON, JA-YONG KOO, Korea Research Institute of Standards and Science — We controlled the ordering between alkanethiol molecules in self-assembled monolayers (SAMs) formed on a Au surface by modifying surface topography of Au films. The ordering between molecules was evaluated using Fourier Transform infrared (FTIR) spectroscopy. A thermal annealing in hydrogen environment removed the nm-scale protrusions from the surface of as deposited Au film resulting in an increase in grain size and a decrease in roughness. This process allowed the alignment of Au atoms in the (111) direction. Together with the aligned Au surface, Au nanoparticles were also prepared as a rough surface with tiny grain size of \( \sim 10 \) nm. The symmetric and asymmetric \( CH_2 \) vibrations in the FTIR spectra showed a larger blueshift from the SAMs on an flatter Au surface. Binding specificity of molecules was examined by Secondary Ion Mass Spectroscopy (SIMS) using a Au pattern formed on a SiO\(_2\)/Si wafer. The molecular signal matched with the Au pattern and the ratio of the signals on Au to SiO\(_2\) was larger than 1000, indicating that the level of non-specific binding was negligible. This method of improving and controlling the ordering between molecules in the SAMs can be applied to sub \( \mu m \) patterns on a SiO\(_2\)/Si wafer.

R1.00239 Detecting Low Levels of Cytochalasin B in 3T3 Fibroblast Cells by Analysis of Electrical Noise Obtained from Cellular Micromotion. DOUGLAS LOVELADY, DAVID RABSON, CHUN-MIN LO, University of South Florida — We performed several micromotion experiments using the electric cell-substrate impedance sensing (ECIS) apparatus on a confluent layer of 3T3 fibroblast cells exposed to differing, low-level amounts of the toxin cytochalasin B. We previously developed a technique to distinguish toxin levels in a single cell type. The noise of the time series extracted from these experiments is characterized by the power spectrum, Hurst exponent, DFA (detrended fluctuation analysis) exponent, first zero and first \( 1/e \) crossing of the autocorrelation function. These measures describe the long- and short-term correlations in the signal, which tell us something about the average behavior of these cells in culture. A change in the behavior of these cells is clearly revealed by an examination of these measures. A principal-component analysis shows a separation of the different toxin levels in the multidimensional space. To our knowledge, this is the most sensitive technique for detecting such a low level of cytochalasin B in 3T3 fibroblast cells.

R1.00240 Trapping Single Molecules With a Solid State Nanopore. MARC GERSHOW, DAVID HOOGHERHEIDE, Harvard University Dept. of Physics, ERIC BRANDIN, Harvard University Dept. of Molecular and Cellular Biology, JENE GOLOVCHENKO, Harvard University Dept. of Physics and School of Engineering and Applied Sciences — We demonstrate a single molecule trap based on a solid state nanopore. A single molecule of DNA is driven through a nanopore by an applied electric field. The passage of the molecule through the nanopore is detected by a decrease in the ionic current through the pore. After the molecule has passed through the pore, we reverse the applied field to recapture the molecule and drive it through the pore again. Upon detection of this second passage, we again reverse the applied field, leading to a third passage through the pore, and so on. Thus the molecule is continually confined by a \( \frac{1}{2} \) potential maintained by active feedback. Upon each passage through the pore, the state of the molecule is electronically interrogated via the measured current blockage. Molecules can be trapped, detected, and analyzed in free solution without any labels or chemical modifications. Repeated electronic interrogation of a single molecule provides a means for greatly enhancing the accuracy with which each molecule can be characterized by a nanopore and allows measurement over time of dynamical properties such as the molecule’s conformation and chemical state.
R1.00241 Subcellular modification of tissue by near-field laser ablation. M. E. REEVES, George Washington University, J. A. HOFFMANN, Applied Physics Laboratory. JASPER NUDAM, BENJAMIN CAMARI, George Washington University, PROTEIN MICROSCOPE COLLABORATION — We report on the development of a near-field approach to MALDI (Matrix-assisted laser desorption and ionization). In this technique analytes embedded in an energy absorbing matrix are ablated from the surface of a sample. In the infrared region, the matrix can be water by exciting the 3-micron vibrational mode of the water molecule. 3-micron wavelength lasers are available with sufficient power to ablate materials of interest, particularly biological samples, however, in most cases the spot size is fairly large, about 40 microns or more, due to the primitive optics available for this wavelength of light. In our laboratory, we have demonstrated near-field focusing of a 3-micron laser to a sub-wavelength spot size with energy sufficient to ablate material from the sample surface. We will review our findings and describe demonstrations of tissue modification by this approach at length scales comparable to the size of a single cell. This approach has the potential to allow the identification and mapping of proteins expressed in intact cells and tissues, which is of great interest as protein expression connects genomic information with the functioning of an organism.

1 W.M. Keck Foundation

R1.00242 Fluorescence spectroscopy investigation and molecular docking simulation of the interaction of β-lactoglobulin A (BLGA) with meso-tetraakis(4-sulfonatophenyl) porphyrin (TSPPP). IVAN SILVA, LORENZO BRANCALON, SAM SANSONE, University of Texas at San Antonio — The interaction of TSPPP and β-lactoglobulin A (BLGA) was studied as a function of pH (6.0-9.0). TSPPP is a dye that is currently in clinical trials for its application in photodynamic therapy of cancer, and BLGA is a well known globular protein. Binding to the protein affects the photochemistry of the dye, hence its potential in clinical applications. Data from TSPPP fluorescence experiments were analyzed and modeled by computational methods. Protein-dye interaction was studied using fluorescence spectroscopy to record the spectral shift (from 643nm to 649nm) to quantitatively bound and free dye with use of Gaussian curve fitting. TSPPP-induced quenching of protein fluorescence determined the binding constant and the number of binding sites through S-V and double-log plots. Fluorescence lifetime characterized the effects of the binding and the location of the binding site through FRET. Unlike the binding of protoporphyrin IX, pH dependence of the TSPPP binding to BLGA is not modulated by the pH conformational change of the protein. Molecular simulation of the docking of TSPPP monomers to BLGA dimers were done using the Arguslab software. Simulations reveal that the interaction is driven by the four negative charges on TSPPP which keep it on the surface of the protein.

R1.00243 The Peyrard-Bishop-Dauxois Model of DNA Dynamics. BOJAN ALEXANDROV, ALAN BISHOP, Los Alamos National Laboratory, ANNY USHEVA, Harvard Medical School, KIM RASMUSSEN, Los Alamos National Laboratory — This presentation details aspects of the rapid development of the connection between the dynamics of double strand DNA, and experimental findings that has occurred in the recent years. We will approach this topic by demonstrating the Peyrard-Bishop-Dauxois model’s ability to provide useful insight on several experimental observations. Specifically, we will focus on the melting behavior of various DNA sequences, and mechanical unzipping through dynamic force spectroscopy. Focusing on viral DNA structures and filters. Interestingly, chaotic behaviors were very rarely observed from analysis.

R1.00244 Design of new inhibitors for H5N1 avian influenza using a molecular dynamics simulation. JIN WOO PARK, WON HO JO, Seoul National University — Recently, there has been a growing interest in the treatment of H5N1 avian influenza. One of the most widely used viral agents is oseltamivir. However, it has been reported that oseltamivir is not as effective as against the neuraminidase subtype N1 as it is against subtypes N2 and N9. In our research we addressed this problem by designing new inhibitors and these altered inhibitor’s binding affinities were calculated. In this study, we introduced chemical groups to the existing oseltamivir, so to fit into the newly discovered cavity in the subtype N1. When the binding strengths of the oseltamivir and the newly designed inhibitors for N1 were calculated to examine the drug efficiency through a molecular dynamics simulation, then compared with each other, it was found that one of the designed molecules exhibited a strong binding affinity, with more than twice the binding strength than that of oseltamivir. Since the aforementioned designed inhibitor appears to have the possibility for oral activity according to the criteria of human oral bioavailability, we propose that the inhibitor is a promising antiviral drug for H5N1 avian influenza.

R1.00245 Phenotypic variability of growing cellular populations. TING LU, Princeton University, TONGYE SHEN, Los Alamos National Lab, MATTHEW BENNETT, PETER WOLYNES, JEFF HASTY, UCSD — The dynamics and diversity of proliferating cellular populations are governed by the interplay between the growth and death rates among the various phenotypes within a colony. In addition, epigenetic multistability can cause cells to spontaneously switch from one phenotype to another. By examining a generalized form of the relative variance of populations and classifying it into intracolony and cross-colony contributions, we study the origins and consequences of cellular population variability. We find that the variability can depend highly on the initial conditions and the constraints placed on the population by the growth environment. We construct a two-phenotype model system and examine, analytically and numerically, its time-dependent variability in both unbounded and population-limited growth environments. We find that in unbounded growth environments the overall variability is strictly governed by the initial conditions. In contrast, when the overall population is limited by the environment, the system eventually relaxes to a unique fixed point regardless of the initial conditions. However, the transient decay to the fixed point depends highly on initial conditions, and the time scale over which the variability decays can be very long, depending on the intrinsic time scales of the system.

R1.00246 Biomolecular Network Simulator: Software for Stochastic Simulations of Biomolecular Reaction Networks on Supercomputers. YAROSLAV CHUSHAK, Biotechnology HPC Software Applications Institute, US Army Medical Research and Materiel Command, BRENT FOY, Wright State University, Dayton, OH 45435, JOHN FRAZIER, Air Force Research Laboratory, Wright-Patterson AFB — At the functional level, all biological processes in cells can be represented as a series of biochemical reactions that are stochastic in nature. We have developed a software tool to simulate complex biochemical networks in order to predict and simulate complex biomolecular reaction networks. Two simulation algorithms - the exact Gillespie stochastic simulation algorithm and the approximate adaptive tau-leaping algorithm - are implemented for generating Monte Carlo trajectories that describe the evolution of a system of biochemical reactions. The software uses a combination of MATLAB and C-coded functions and is parallelized with the Message Passing Interface (MPI) library to run on multiprocessor architectures. We will present a brief description of the Biomolecular Network Simulator software along with some examples.

3 This work was supported by funds provided by the DoD High Performance Computing Modernization Program (HPCMP) and by the Air Force Office of Scientific Research (AFOSR).

R1.00247 Determining behaviors of biological networks with dynamic logic method. SUPING LYU, Medtronic Inc — Dynamic logic method was used to study dynamic behaviors of some network motifs. This method combines logic operations and kinetic parameters of biochemical reactions (response or delay times). The analysis is simple because it is pure symbolic operation without numerical calculation. We proved in general that if networks are cycles with an odd number of suppression interactions, the cycles will oscillate. Delay times are necessary for oscillatory networks. If delay times are zero, the systems stay at stable states. If there is an even number of suppression interactions, the cycles have two stable states. Signal travel in chain-like networks was also studied. The depths of travel depend on the pulse width of signals and the filters of chains. Same signals with different pulse widths can have different biological responses (one stimulation to multiple responses). When pulsive signal travel in cycles, they can remain to be pulses, die, or become flat (all active) depending on the filters of cycles. The coupled cycles have complicated behaviors that are determined by their intrinsic structures and filters. Interestingly, chaotic behaviors were very rarely observed from analysis.
R1.00248 Active Dynamics of Microtubule Bundles, ASSAF ZEMEL, Department of Neurobiology, Physiology and Behavior, University of California, Davis 95616, USA, ALEX MOGILNER, Department of Mathematics and Department of Neurobiology, Physiology and Behavior, University of California, Davis 95616, USA — Microtubule bundles play a central role in a variety of dynamical processes in cells such as cell division, neural growth and blood platelet formation. These processes are driven by the activity of molecular motors that exert sliding forces on the microtubules. In such bundles, motor proteins may crosslink two or more filaments, forming discrete clusters of microtubules whose dynamics is governed by a balance of the motor-generated forces. The connectivity of these microtubule-motor complexes is an essential property of the bundle and dictates its dynamics. We present a systematic computational study of these microtubule bundles based on force-balance computer simulations as well as a simplified analytical theory. This allows us to calculate the characteristic times of microtubule sorting and spreading, as well as the effective diffusion constants and drift coefficients as a function of the microtubule density and the polarity fraction of the microtubules. Application of our theory in the study of blood platelet formation is presented.

R1.00249 Preliminary comparative studies of Thermus aquaticus resilience to thermal and microwave heat input, KONRAD KABZA, Southeastern Louisiana University, KAREN GEORGE, Southeastern Louisiana University, STELLA VON MEER, ARMIN KARGOL, Loyola University New Orleans — Thermus aquaticus was grown using existing ATCC protocol. Bacteria were cultured in large batches and each batch partitioned into usable 250 mL aliquots. These samples were then tested using identical parallel experiments, one heated with a traditional thermal heat source, while the other was irradiated with a 2.45 GHz conventional microwave oven. Relative growth of the Thermus aquaticus was measured using UV visible spectroscopy at 400 nm. Multiple runs of the same experiments were averaged and the growth data for both modes of energization plotted. A unique low microwave exposure apparatus with a flow-through cell will be described and the entire experimental setup discussed.

R1.00250 Electroshock weapons can be lethal! MARJORIE LUNDQUIST, Bioelectromagnetic Hygiene Institute, P. O. Box 11831, Milwaukee, WI 53211-0831 USA — Electroshock weapons (EWs)—stun guns, tasers, riot shields—are electroconductive devices designed to safely incapacitate healthy men neuromuscularly, so they are called nonlethal or less-lethal. EW firms seeking large nonmilitary markets targeted law enforcement and corrections personnel, who began using EWs in prisons/jails and on public patrol in 1980 in the USA. This shifted the EW-shocked population from healthy soldiers to a heterogeneous mix of both sexes, ages 6-92, in a wide variety of health conditions! An EW operates by disrupting normal physiological processes, producing transient effects in healthy people. But if a person’s health is sufficiently compromised, the margin of safety can be lost, resulting in death or permanent health problems. 325 people have died after EW shock since 1980. Did the EW cause these deaths? Evidence indicates that EWs do play a causal role in most such deaths. EWs can be lethal for people in diabetic shock (hypoglycemia), which may be why Robert Dziekanski—a Polish immigrant to Canada—died so quickly after he was tasered at Vancouver Airport: not having eaten for over 10 hours, he likely was severely hypoglycemic. The EW death rate in North America is 30 times higher than need be, because EW users have not been properly trained to use EWs on a heterogeneous population safely! 1 J. Clinical Engineering 30(3):111(2005).

R1.00251 Analytic Thermodynamic Calculations for an Immobilized Molecule under Poisson-Boltzmann Interactions using a Spheroidal Geometry, JOAQUIN AMBIA-GARRIDO, MONTGOMERY PETTITT, UNIVERSITY OF HOUSTON TEAM — The change in some thermodynamic quantities such as Gibb’s free energy, entropy and enthalpy of the binding of a particle tethered to a surface or particle are analytically calculated. These particles are considered ellipsoids and submerged in a liquid. The ionic strength of the media allows the linearized version of the Poisson-Boltzmann equation (from the theory of the double layer interaction) to properly describe the interactions between an ion penetrable spheroid and a hard plate. We believe that this is an adequate model for a DNA chip and the predicted electrostatic effects suggest the feasibility of electronic control and detection of DNA hybridization and design of chips underlying avoiding the DNA folding problem.

R1.00252 ABSTRACT WITHDRAWN —

R1.00253 Kinesin motor protein as an electrostatic ratchet machine, GEORGE TSIRONIS, University of Crete and FORTH, ALEIX CIUDAD, JOSE MARIA SANCHO, University of Barcelona — Kinesin and related motor proteins utilize ATP fuel to propel themselves along the external surface of microtubules in a processive and directional fashion. We show that the observed step-like motion is possible through time varying charge distributions furnished by the ATP hydrolysis circle while the static charge configuration on the microtubule provides the guide for motion. Thus, while the chemical hydrolysis energy induces appropriate local conformational changes, the motor translational energy is fundamentally electrostatic. Numerical simulations of the mechanical equations of motion show that processivity and directionality are direct consequences of the ATP-dependent electrostatic interaction between the different charge distributions of kinesin and microtubule. Treating proteins as continuous dielectric media and using a Green’s function formalism we find analytical expressions for the electrostatic energy in the vicinity of the protein surfaces. We calculate the Bjerrum length in the interior of the protein and analyze the different charge distributions of kinesin and microtubule. We apply these results to kinesin and estimate the pure electrostatic ATP-ADP interaction to be larger than 2k T.

R1.00254 Efficiency optimization of the Buttiker-Landauer Heat Engine, RONALD BENJAMIN, RYOICHI KAWAI, University of Alabama at Birmingham — We study the energetic efficiency of a Brownian heat engine driven by spatially inhomogeneous temperature in presence of periodic potential, via Molecular Dynamics (MD) simulation as well as by numerically solving the inertial Langevin equation. We explore various potential shapes and different locations of the temperature boundary to identify the parameter regime in which the efficiency can be optimized. However the irreversible heat flow from the hot to the cold reservoir due to the particle’s kinetic energy severely limits the efficiency and is not very sensitive to variations of the parameters. We also investigated the heat engine when it works with maximum power and found that the efficiency is much lower than that of the corresponding endoreversible engine.

R1.00255 The anomalous polarization property in laser diode, TZU FANG HSU, YEN CHUN LIN, YUNG HSUN CHEN — We have experimentally found some anomalous polarization property in laser diode (LD). As laser beam was merely passing through a polarizer, the polarization curve acted as normal cosine function which obeyed the behavior of linear polarization, fitting the property of LD. However, the polarization curve that linear polarized beam reflected by a glass plate became the W shape, which is much more different to the curve of linear polarized light. By experimentally demonstrated, it is found that this anomalous curve was revealed as the linear polarized laser beam experienced the condition of second reflection, so that the curve of reflecting by mirror was normal cosine function and by prism was also the W shape.
R1.00256 Anomalous diffusion and passage time distributions of microscopic particles through biological layers¹. M. GREGORY FOREST, University of North Carolina at Chapel Hill, CHRISTEL HÖHENEGGER, Courant Institute, New York University, SCOTT MCKINLEY, Duke University, LINGXING YAO, University of North Carolina at Chapel Hill — The field of passive microrheology was launched by Mason and Weitz in 1997, and has subsequently advanced in a variety of experimental and theoretical directions. The original aim is to infer viscoelastic properties from mean-squared displacement statistics of Brownian particles (beads) dispersed in the material. Extensions to bead-bead correlations have been advanced to screen local particle-material chemical potentials. The experimental measurements are equally, if not more so, ideal for characterizing the anomalous diffusive transport properties of soft matter, which are fundamental to pathogen or drug carrier diffusion through biological layers. Direct and inverse modeling and simulation tools will be presented, together with an evaluation of how well mean squared displacement serves as a proxy for passage time distributions.

¹Research supported by NIH, NSF, and AFOSR.

R1.00257 Test of the noise-induced nonequilibrium kinetic focusing of voltage-gated ion channels¹. ARMIN KARGOL, Loyola University New Orleans, KONRAD KABZA, Southeastern Louisiana University, STELLA VON MEER, Loyola University New Orleans — It has been postulated [1] that voltage-gated ion channels can be focused into specific conformational states by application of fluctuating voltages, such as dichotomous noise. We conducted an experimental test on Shaker K+ channels. We applied the dichotomous noise, reproducing the conditions in [1] as close as is experimentally feasible. We also varied the frequency and the amplitude of the dichotomous noise within a certain range. We observed that in some cases, for intermediate noise frequencies (1-2 kHz) and large amplitudes, the probability for intermediate states in the Markov model of the ion channel gating kinetics can be significantly increased above the maximal value for any static voltages. However, so far the scale of the focusing effect observed experimentally is smaller than the numerical simulations predict.

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R1.00258 Wavelet-based protocols for ion channel electrophysiology¹. ARMIN KARGOL, Loyola University New Orleans — Ion channel gating kinetics is usually represented as a discrete Markov model whose input is the applied membrane voltage and the output is the ionic current. A current paradigm in experimental ion channel electrophysiology is to subject the channels to static voltages, which results in equilibrium or near-equilibrium conditions. We implement a new type of rapidly fluctuating voltage inputs that drive ion channels into nonequilibrium distributions. We discuss an algorithm for generating time-varying voltage inputs as a composition of wavelets, which allows optimization of spectral and temporal properties of voltage inputs for specific purposes, such as model selection. The outputs of channel Markov models for the Shaker K+ channels are compared to the experimental data (whole cell ionic currents) recorded from these channels.

¹This work was partially supported by the Cottrell College Science Award (CC6481) from Research Corporation.

R1.00260 The Detection of Protein via ZnO Resonant Raman Scattering Signal. GUIYE SHAN, GUOLIANG YANG, Drexel University, SHUANG WANG, YICHUN LIU, Northeast Normal University — Detecting protein with high sensitivity and specificity is essential for disease diagnostics, drug screening and other application. Semiconductor nanoparticles show better properties than organic dye molecules when used as markers for optical measurements. We used ZnO nanoparticles as markers for detecting protein in resonant Raman scattering measurements. The highly sensitive detection of proteins was achieved by an antibody-based sandwich assay. A probe for the target protein was constructed by binding the ZnO/Au nanoparticles to a primary antibody by electrostatic interaction between Au and the antibody. A secondary antibody, which could be specifically recognized by target protein, was attached to a solid surface. The ZnO/Au-antibody probe could specifically recognize and bind to the complex of the target protein and secondary antibody. Our measurements using the resonant Raman scattering signal of ZnO nanoparticles showed good selectivity and sensitivity for the target protein.

R1.00261 Influence of dissolved gasses on hydrophobic interaction at different length-scales¹. ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University (VCU), 1001 West Main Street, Richmond, VA 23284-2006, D. BRATKO², University of California at Berkeley — Despite widespread experimental evidence of the influence of dissolved gases on hydrophobic interaction, the mechanism of observed effects are still unknown. We present direct calculations of the hydrophobic force between model hydrophobic surfaces in the presence and absence of dissolved gases, and varying surface separation up to 4 nm. We monitor gas adsorption at molecular resolution inaccessible to experiments. We find insignificant gas adsorption, confined to the first molecular layer, and no dependence of the width of the perturbed water layer on the amount and type of dissolved gas. The results offer a molecular-level interpretation for the lack of influence of dissolved gas on the short-range hydrophobic force, a finding that is consistently reported in experiments that show a dramatic gas effect at long-range, but minimal at short-range or in determining the adhesion force or interfacial energy. Finally, a coarse-grained approach is discussed to deal with apparent non-equilibrium effects at longer-range and implications to biological systems and nanoscience.

¹supported by NSF.
²2nd affiliation: Department of Chemistry, VCU
R1.00262 Imaging Applications of the Geant4 Simulation Toolkit. JOSEPH PERL, Stanford Linear Accelerator Center — Geant4 is a toolkit for the simulation of the passage of particles through matter. While Geant4 was originally developed for High Energy Physics (HEP), applications now include Nuclear, Space and Medical Physics. Medical applications of Geant4 in North America and throughout the world have been increasing rapidly due to the overall growth of Monte Carlo use in Medical Physics and the unique qualities of Geant4 as an all-particle code able to handle complex geometry, motion and fields with the flexibility of modern programming and an open and free source code. Many developers of imaging technology use Geant4 by way of GATE, the Geant4 Application for Emission Tomography, which comes around Geant4 to simplify use and add imaging features, while other imaging developers use Geant4 directly. This talk will provide an overview of these applications, with a focus on how Geant4’s unique qualities, such as its support for moving geometries and electric and magnetic fields, are applied to medical imaging.

R1.00263 Sequence effects on the translocation of heteropolymers through a small channel1. MICHEL G. GAUTHIER, GARY W. SLATER, University of Ottawa — Using a recently developed Monte Carlo algorithm and an exact numerical method, we calculate the translocation probability and the average translocation time for charged heteropolymers driven through a nanopore by an external electric field. The heteropolymer chains are composed of two types of monomers (A and B) which differ only in terms of their electric charge. We present an exhaustive study of chains composed of 8 monomers by calculating the average translocation time associated with the 256 possible arrangements for various ratios of the monomer charges ($\lambda_A / \lambda_B$) and electric field intensities, $E$. We find that each sequence leads to a unique value of the translocation probability and time. We also show that the distribution of translocation times is strongly dependent on the three parameters $\lambda_A$, $\lambda_B$ and $E$. Finally, we present results that highlight the effect of having repetitive patterns by studying the translocation times of various block copolymer structures for a very long chain composed of N = 218 monomers (with the same number of A and B monomers).

1This work was supported by a Discovery Grant from the Natural Sciences and Engineering Research Council of Canada (NSERC) to GWS and by scholarships from the Ontario Graduate Scholarship Program (OGS) and the University of Ottawa to MGG.

R1.00264 INSULATORS AND DIELECTRICS —

R1.00265 The new single crystals with alpha-quartz structure obtained by hydrothermal method , MICLAU MARINELA, BUCUR RAUL, POENAR MARIA, VLAZAN PAULINA, GROZESCU IOAN, Condensed Matter Research Department, National Institute R&D Electrochemistry and Condensed Matter, Pautuliu Andronescu 1, Timisoara, Romania, MUSCUTARIU IOAN, Baldwin-Wallace College, Berea, Ohio 44017-2088, U.S.A., MICLAU NICOLAE, “POLITEHNICA” University of Timisoara, Bd. Vasile Parvan, nr.2, Romania, INCERC TEAM, BALDWIN-WALLACE COLLEGE TEAM, POLITEHNICA UNIVERSITY TEAM — Interest of Si1-xGeO2 single crystal with alpha-quartz structure is connected to improvement of electromechanical coefficients and rise of alpha - beta phase transition of quartz one. Growth of alpha - Si1-xGeO2 single crystal was realized by a hydrothermal method of temperature gradient in autoclaves, made from Cr-Ni alloys. Nutrient material was prepared from synthetic quartz and placed in the bottom of autoclaves. There was loaded GeO2 powder additive in proportions to quartz nutrient. Single crystals were investigated by electron microscope analysis, X-ray diffraction and atomic force microscopy. The most important result, which was obtained during the investigations, is an experimental proof of growth of Si1-xGeO2 solid solutions single crystals (with quartz structure) under the hydrothermal conditions. The present results thus open the possibility to tune the piezoelectric properties of these materials by varying the chemical composition.

R1.00266 Anomalous relaxation of damped graded elastic lattices1, M.I. ZHENG, Chinese University of Hong Kong, J.J. XIAO, Hong Kong University of Science and Technology, K. YAKUBO, Hokkaido University, K.W. YU, Chinese University of Hong Kong — We study the relaxation of harmonic vibrational excitations of damped graded lattices with a mass gradient. In the previous work, no damping was considered [1]. In this work, we re-examine the vibrational modes in a rigorous quasi-normal mode approach. It is shown that both the damping positions and boundary conditions can affect the relaxation spectrum. Moreover, there exists a dip at the gradon transition frequency for one-dimensional (1D) damped chains with damping at two ends or on all the sites. In two-dimensional (2D) orthogonally graded squared lattices (OGSL), there exist a dip and a peak at the two boundary frequencies of soft-hard gradon region. Moreover, the dip and peak structures in the relaxation spectrum can be explained by the anomalous gradon wavefunctions.

1Supported by RGC and JSPS.

R1.00267 Density of States of Silicon, Silicon Dioxide, Silicon Nitride and Silicon Carbide1 , HONG DONG, A.R. CHOIRASIA, Department of Physics, TAMU-Commerce, S.D. DESHPANDE, Department of Physics, Amravati University, India — The density of states of Si, SiC, Si3N4 and SiO2 have been studied using a DFT computational approach implemented in CRYSTAL06. This code employs linear combinations of Gaussian type functions to represent single particle wave functions. The Becke exchange and Lee, Yang and Parr correlation have been employed. The atomic basis sets with a polarization function have been optimized for each configuration in these materials. The unit cell parameters have also been optimized. The density of states in the valence and conduction bands have been computed in each case. The projected density of states of the constituents has also been computed. The band gap has been calculated for these materials. These values are compared with the available experimental data. The correlation between the electronic polarizability and the Auger parameter determined previously from x-ray photoelectron spectroscopy will be presented.

1Work supported by Research Corporation and Organized Research, TAMU-Commerce.

R1.00268 Spectral representation theory of graded composite materials , K.L. CHAN, C.M. KWOK, K.W. YU, The Chinese University of Hong Kong — In graded composite materials, the physical properties can vary continuously in space and it may give different physical phenomena when compared with homogeneous materials. The Bergman-Milton spectral representation is a rigorous mathematical formalism to express the effective dielectric constant of nongraded composite materials [1]. In this study, we consider a material (rather than microstructure [2]) graded composites, and generalize the Bergman-Milton spectral representation to extract the spectral density function for the effective dielectric constant of this graded composite material in the frequency domain [3]. Analytic and numerical solution will be presented for graded films and graded spheres.


R1.00269 Optical Trapping Forces from Electric Fields Inside Dielectric Materials1 , DOUGLAS BONESSI, KEITH BONIN, Wake Forest University, THAD WALKER, University of Wisconsin, Madison — We developed a method for computing forces from internal electric fields. The internal fields are found using discrete dipole approximation (DDA) and finite difference time domain (FDTD) approaches and the results are compared. We are interested in the results from an optical trapping viewpoint, though other simulations are used for benchmarks. This method can handle arbitrary input beams and particle sizes and shapes. We hope to report on similar calculations to calculate optical torques on birefringent particles in the Mie size regime.

1This research was supported by a grant from Research Corporation
R1.00270 DFT Ab initio Calculation of Vibrational Frequencies in AsSe glass, KESHAV SHRVASTAVA, HASAN KASSIM, AHMAD NAZRUL ROSLI, University of Malaysia, JABATAN FIZIK COLLABORATION — By using DFT double zeta wave functions, we calculated the structure, bond length (picometer, pm), frequencies (intensities) (degeneracy) for various clusters of arsenic selenide. Our results are as follows. (i) AsSe(diatomic) bond length 216 pm, 244.0 (1/cm). (ii) AsSe(2+) bond length 228.5 pm, frequencies 27.6 (1.9) and 387.6 (4.3). (iii) AsSe(2+) bond length 234.3 pm, As-As 223.3 pm, frequencies 237.3 (2.4) and 332.4 (0.05) (1/cm). (iv) AsSe(2+) bond length 238.4 pm, frequencies 107.5 and 296 (weak) (1/cm). (v) AsSe (square) bond length 250.2 pm, 58.5 (0.04), 241.3 (5.9) (1/cm). (vi) AsSe (triangular) bond length 231.2 pm, 75.9 (0.003), 103.5 (1.26) [2], 350.9 (33.2) [2]. From this study we identify that linear As-Se-As for which the calculated frequency is 27.6 (1/cm) is in agreement with the data of Nemamich, Phys. Rev. B 16, 1659 (1977). J. C. Phillips et al Phys. Rev B 21, 5724 (1980). We have successfully calculated several vibrational frequencies accurately which agree with the Raman data.


R1.00271 Raman spectroscopy of multiferroic trigonal boracite Cs$_3$B$_2$O$_5$Cl$^-$, MILKO ILIEV, VIKTOR HADJIEV, Texas Center for Superconductivity at the University of Houston, MARIA-EUGENIA MENDOZA, Instituto de Fisica, Universidad Autonoma de Puebla, Puebla, Mexico, JORDI PASCUAL, Institut Catal`a de Nanotecnologia (ICN) and Departament de Fisica, Universitat Autonoma de Barcelona, Barcelona, Spain. — Raman microscopy was applied to study the polarized Raman scattering from untwinned domains of Cs$_3$B$_2$O$_5$Cl$^-$ (Co-Cl) in the trigonal, R3$_c$, ferroelectric phase. The symmetry (A$_1$ or E) and mode polarization (LO or TO) for all observed Raman lines were determined from comparison of the spectra measured in several scattering configurations. It was found that as a rule the TO-LO splitting is small or negligible. A group of A$_1$ modes, characterized by a quasi-one-component Raman tensor, was tentatively assigned to stretching vibrations of Cl, O, or B along the trigonal axis, which in this material is parallel to the ferroelectric polarization direction.

1 Supported by the State of Texas through Texas Center for Superconductivity at the University of Houston

R1.00272 Infrared spectroscopy of Dysprosium doped KPb$_2$Br$_5$ and KPb$_2$Cl$_5$, PETER AMEDZAKE, EI BROWN, UW HOMEIMERICH, Hampton University, SUDHIR TRIVEDI, Brimrose Corporation of America, JOHN ZAVADA, US Army Research Office — The infrared optical properties of rare earth doped crystals with narrow phonon spectrum (< 300 cm$^{-1}$) remains of current interest for applications in IR solid-state gain media. The maximum phonon energies of KPb$_2$Cl$_5$ and KPb$_2$Br$_5$ are only ~200 cm$^{-1}$ and ~150 cm$^{-1}$, which reduce non-radiative decay through multi-phonon relaxations. In this work, we present spectroscopic results of Dy: KPb$_2$Cl$_5$ and Dy: KPb$_2$Br$_5$ for possible applications in mid-infrared gain media. The investigated materials were grown by vertical Bridgman technique. Dy: KPb$_2$Cl$_5$ and Dy: KPb$_2$Br$_5$ exhibited characteristic Dy$^{3+}$ absorption bands in the visible and infrared regions. Optical excitation at ~800 nm resulted in the observation of a broad 4-5 $\mu$m mid-IR emission ($^{6}H_{11/2} \rightarrow ^{6}H_{3/2}$) at room temperature. The mid-IR emission lifetime was measured to be ~5.5 ms for Dy: KPb$_2$Cl$_5$ and ~3.8 ms for Dy: KPb$_2$Br$_5$, respectively. Based on temperature dependent lifetime studies and Judd-Olfet calculations, the emission quantum efficiencies for the 4-5 $\mu$m bands were estimated to be near unity. More details on the IR optical properties of Dy: KPb$_2$Cl$_5$ and Dy: KPb$_2$Br$_5$ will be presented at the conference.

R1.00273 Mid-infrared Emission and Energy Transfer Properties of Sensitized Rare Earth Ions in KPb$_2$Cl$_5$, ALTHEA BLUIETT, ERICA PINKNEY, Elizabeth City State University, EI BROWN, UW HOMEIMERICH, Hampton University, SUDHIR TRIVEDI, Brimrose Corporation of America, JOHN ZAVADA, US Army Research Office — Mid-infrared emission (4-5 $\mu$m) originating from the first excited state of Pr$^{3+}$ and from the first excited state of Nd$^{3+}$ were generated by means of Yb$^{3+}$ and Tm$^{3+}$ sensitization, respectively. The mechanisms involved in sensitizing Pr$^{3+}$ and Nd$^{3+}$ ions were determined by studying the decay kinetics of the $^2F_{5/2} \rightarrow ^2F_{7/2}$ transition of Yb$^{3+}$ and the $^4F_4 \rightarrow ^2H_6$ transition of Tm$^{3+}$ under 970 nm and 1750 nm laser excitation, respectively. It was observed that the emission lifetime of the $^2F_{5/2} \rightarrow ^2F_{7/2}$ transition and the $^4F_4 \rightarrow ^2H_6$ transition were reduced considerably in the presence of the activator ions Pr$^{3+}$ and Nd$^{3+}$, respectively. Strong 4-5 $\mu$m emission from Pr$^{3+}$ and Nd$^{3+}$ were observed in Yb, Pr: KPb$_2$Cl$_5$ and Tm, Nd: KPb$_2$Cl$_5$, respectively. These findings indicate that significant energy transfer was transpired. Concentration dependent studies will be conducted to ascertain the dopant concentrations for efficient MIR emission.

R1.00274 Rectifying Current-Voltage Characteristics of BiFeO$_3$/Nb-doped SrTiO$_3$ Heterojunction, HAO YANG, H.M. LUO, Superconductivity Technology Center, Los Alamos National Laboratory, H. WANG, Dept. of Electrical and Computer Engineering, Texas A&M University, D.M. FELDMANN, Q.X. JIA, Superconductivity Technology Center, Los Alamos National Laboratory — Epitaxial c-axis oriented BiFeO$_3$ (BFO) thin films were deposited on (001) Nb-doped SrTiO$_3$ (Nb-STO) substrates by pulsed laser deposition. Introducing Bi vacancies causes the BFO thin film to evolve to a p-type semiconductor and form a p – n heterojunction with n-type semiconductor Nb-STO. The current density vs voltage ($J$ – $V$) and capacitance vs voltage ($C$ – $V$) characteristics of the heterojunction were investigated. A typical rectifying $J$ – $V$ effect was observed with a large rectifying ratio of 5x10$^4$. Reverse $C$ – $V$ characteristics exhibit a linear 1/C$^2$ vs $V$ plot, from which a built-in potential of 0.6 V is deduced. The results show a potential application of BFO/Nb-STO heterojunction for oxide electronics.

R1.00275 Wet-chemistry synthesis and dielectric properties of pure and Rb and V doped Cs$_2$Nb$_2$O$_6$$_{11}$, JIANJUN LIU, Department of Physics, University of Nebraska at Omaha, ROBERT SMITH, Department of Chemistry, University of Nebraska at Omaha, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha — Cs$_2$Nb$_2$O$_6$$_{11}$ (CNO) is an antiferroelectric compound whose single crystal structure and antiferroelectric properties have been recently reported [1]. It has a space group of Pnna and a phase transition temperature at 165 °C. In this study we synthesized CNO powdered samples, both pure and doped with rubidium and vanadium, by using a wet-chemistry method. Dielectric measurements showed that the phase transition temperature shifted with the doping. We analyzed the mechanism of this antiferroelectric phase transition based on the observed results. [1] Robert W. Smith, Chunhua Hu, Jianjun Liu, Wai-Ning Mei, Kuan-Jiuh Lin, J. Solid State Chem. 180 (2007) 1193-1197.

1 This work was supported by the Nebraska Research Initiative.

R1.00276 Effect of Pressure on the Atomic and Electronic Structure of Hexagonal YMnO$_3$, ZHIGLIANG CHEN, TREVOR TYSON, New Jersey Institute of Technology, SUNGBAEK KIM, SANG-WOOK CHEONG, Rutgers University — The multiferroic hexagonal system YMnO$_3$ is known to possess a significant polarization at room temperature. To understand the mechanism behind the polarization, we conducted high pressure x-ray diffraction measurements for pressures between ambient and 20 GPa. The powder diffraction data were refined to obtain the atomic level structure as a function of pressure. The pressure dependence of resistivity at room temperature (for pressures up to -6 GPa) was determined. Complementary density functional calculations were conducted to correlate the changes in electronic structure and polarization with the observed changes in atomic structure with pressure.

1 This work is supported by DOE Grant DE-FG02-07ER46402.
R1.00277 Acoustic and Optical Properties of Er$^{3+}$-doped LiNbO$_3$. ALEM TEKLU, NARAYANAN KUTHIRUMMAL, DANIEL MORRALL, JAY DANDREA, College of Charleston — Elastic constants of pure and Er$^{3+}$-doped lithium niobate (LiNbO$_3$) single crystals have been determined using resonant ultrasound spectroscopy (RUS). When comparing the elastic constants for pure and doped LiNbO$_3$ crystals, the bulk modulus was found to increase by 5.2% after doping. Also the elastic constants were compared. $C_{11}$ decreased by 4%, $C_{12}$ increased by 18% and $C_{44}$ increased by 16.6%. The surface-doping explains the decrease in elastic constant in only one direction. The presence of Er$^{3+}$ ions on the surface of LiNbO$_3$ has been monitored using photoacoustic spectroscopy. The photoacoustic spectrum revealed very weak absorptions corresponding to $4F^{7/2}$, $4F^{9/2}$ and $2H^{11/2}$ levels of Erbium, indicating the presence of Erbium.

R1.00278 Dielectric response in potassium tantalite/potassium niobate multilayers, M. E. REEVES, SHUOGANG HUANG, George Washington University, JENNIFER SIGMAN, Sandia national Laboratory, DAVID NORTON, University of Florida, HANS CHRISTEN, Oak Ridge National Laboratory — We report measurements of the dielectric response of thin-film multilayers of potassium tantalite/potassium niobate. The measurements were made by evanescent-probe microscopy, a technique that is quite sensitive to material placed in the near-field proximity of the sample probe. The measurements were performed at a frequency of 1.7 GHz with the electric field polarized perpendicular to the plane of the film. Our results show that there are two distinct phase transitions. The first coincides with a structural transition in the material and indicates the onset of coupling between the potassium niobate layers. The transition moves to higher temperature as the spacing between the layers in increased. A second lower temperature transition indicates the onset of anti-ferroelectric ordering in the sample. The temperature of this transition is nearly independent of layer thickness and is not connected with a structural transition. The mechanism for the transitions will be discussed and data measured on asymmetric multilayers will be presented.

R1.00279 Anomalous size dependence of inverse participation ratio of localized eigenfunctions in graded elastic lattices$^1$, M.J. ZHENG, Chinese University of Hong Kong, M. GODA, Niigata University, K. YAKUBO, Hokkaido University, K.W. YU, Chinese University of Hong Kong — Recently, we studied harmonic vibrational excitations in graded elastic lattices [1]. It is found that the eigenfunctions exhibit a transition from extended phonon states to localized gradon states when the frequency is increased beyond a critical frequency called the gradon transition frequency. At the same time, the inverse participation ratio (IPR) can exhibit a rapid increase at gradon transition. This unusual behavior prompts us to study the size dependence of the IPR of gradon wave function. A quantum analogue is established for the hump structure at the gradon front, via the fact that the probability of a quantum particle is inversely proportional to its volume. In this way, the envelope function can be determined analytically, and matches the gradon wave function quite well. We find that the size $N$ dependence can be captured by the relation: \( \text{IPR} = C_1 \log(N) + C_2 \), where $C_1$ and $C_2$ are constants. The interpretation is important in the understanding of a wide variety of properties of graded systems.

$^1$Supported by RGC and JSPS.

R1.00280 SUPPLEMENTARY ABSTRACTS —

R1.00281 Physics and Operational Research: measure of uncertainty via Nonlinear Programming. YASSER A. DAVIZON-CASTILLO$^1$, Arizona State University — Physics and Operational Research presents an interdisciplinary interaction in problems such as Quantum Mechanics, Classical Mechanics and Statistical Mechanics. The nonlinear nature of the physical phenomena in a single well and double well quantum systems is resolved via Nonlinear Programming (NLP) techniques (Kuhn-Tucker conditions, Dynamic Programming) subject to Heisenberg Uncertainty Principle and an extended equality uncertainty relation to exploit the NLP Lagrangian method. This review addresses problems in Kinematics and Thermal Physics developing uncertainty relations for each case of study, under a novel way to quantify uncertainty.

$^1$Department of Industrial Engineering

R1.00282 Physics of Large Scale Production Systems under Uncertainty. YASSER A. DAVIZON-CASTILLO, Department of Industrial Engineering, Arizona State University — Large Scale Production Systems (LSPS) are analyzed from the physics perspective based on the measure of uncertainty. A novel approach to quantify uncertainty is presented using Little’s law and Uncertainty Inequalities in Throughput and Work in Process. The extended version of an Uncertainty equality relation is used to measure the levels of uncertainty in the LSPS in a Nonlinear Programming context. Conservation of Energy Principle is used to determine the measure of uncertainty overall the system. The main contribution is the analogy from the physical phenomena to a LSPS arena using the Conservation of Energy Principle.

R1.00283 A High-resolution Rapidly-updated Meteorological Data Analysis System for Aviation Applications. CHI SHING LAU, MING CHUNG CHU, JONES TSZ-KAI WAN, The Chinese University of Hong Kong, PING WAH LI, Hong Kong Observatory — We present our work on the recent development of a high spatial- and temporal-resolution meteorological data analysis system for the identification and monitoring of mesoscale to microscale weather phenomena over the Hong Kong International Airport (HKIA) and its vicinity. The system can be updated minutely with a horizontal resolution of 150 m. The system is adapted from the Local Analysis and Prediction System (LAPS) from NOAA. Apart from conventional data such as automatic weather stations, wind profilers and satellite observations, automatic aircraft reports (AMDAR), LIDARs and Terminal Doppler Weather Radar (TDWR) data are ingested into the system. The LIDAR and TDWR data are complimentary to each other so that wind field can be identified in both clear and convective weather. Ingesting the above data into the system helps generate a comprehensive 3-dimensional structure of the atmosphere over the airport and nearby airspace. The analysis system would also be useful for newcast aviation-related weather after integrating with numerical weather prediction models. Several cases such as land-sea breeze, gust front and tropical cyclone are discussed. Our results could bring significant insights into aircraft safety and air traffic efficiency to the flights operating at other airports over the world.

R1.00284 Simulating a charged spherical pendulum in time-varying electric and magnetic fields$^1$, MARK WELLONS, FRANK KING, TODD MCALPINE, The College of Wooster — We simulate and analyze the dynamics of a charged spherical pendulum in time-varying electric and magnetic fields. The time-varying electric field is directed perpendicular to the gravitational field and serves as a driving force for the pendulum. The time-varying magnetic field is directed parallel to the gravitational field and serves to deflect the motion of the pendulum. We analyze the dynamics of the system to determine the conditions for which chaotic behavior is observed. We also include viscosity to look for strange attractors. The equations of motion are integrated using Objective C and the graphical user interface, including the three dimensional graphical representation of the system, is developed using Cocoa.

$^1$We thank NSF REU DMR-0649112 and The College of Wooster for their support.

R1.00285 POST-DEADLINE ABSTRACTS —
R1.00286 Electrode-side impedance nonlinearity in polycarbazole bioelectrodes quantifiable by a quaternion formalism, M. OVAHIA, D.H. ZAVITZ, UIC, Y.P. KAYNAMURA, J.F. RUBINSON, Georgetown — Nonlinear response to sinusoidal electrification is a phenomenon rarely observed for conductive interfaces. We report nonlinear response as an electrode phenomenon in a conjugated polymer electrode polycarbazole. While other semiconductors manifest an impedance quantifiable in the complex field (e.g., Warburg where complex $Z = Z_{W}^{\infty}$ and resistive with $Z = Z_{R}$ [HI-Hallblert]) the polycarbazole manifests no definable impedance due to essential nonlinearity. There is no description available for this form of pseudoconductivity. We introduce a quaternion formalism $Z_{Cg} = ai + bj + ck + dl$ [where $a, b, c, d$ are real and $i^2 = j^2 = k^2 = -1$ and $j = i$] that successfully describes all conductivity ($c = d = 0$) and pseudoconductivity presently known as a normed ring, and reduces to the complex field for conductivity. In this formalism, the normalized impedance of a capacitor is $Z = i$, the experimentally determined polycarbazole pseudoimpedance $Z_{Cg} = k$, that of a resistance is $Z = 1$ and that of the $Z_{W}^{\infty} = v/\sqrt{i}$. The non-Abelian character of $Z_{Cg}$ implies that the Onsager relation fails for some interfaces. Remarkably, certain Kramers-Kronig relations (Hilbert transformation in not only the complex but also the $[j, k]$ plane) still hold for certain experimental setups. Computation of the energy integral $\int_{DEdt}$ reveals that charge transport is lossless, similar to conduction in an ordinary capacitor.

R1.00287 Static And Dynamic Studies In Nonyloxycyanobiphenyl (9ocb) Confined To Anopore Membranes, SERGIO DIEZ BERART, Kent State university, MIGUEL ANGEL PEREZ JUBINDO, DAVID O. LOPEZ, M. ROSARIO DE LA FUENTE, JOSEP SALUD — We analyze and compare the static and dynamic properties of alkoxycyanobiphenyl (9OCB). This compound exhibits an I-N-SmA phase sequence. After confining into Anopore structures several phenomena can be seen: Both phase transitions change in their nature, $C_{p}$ peaks becoming lower, broader and shifted down in temperatures. A possible first-to-second order transition could be determined for the N-SmA. There develops a surface induced nematic layer that becomes larger when temperature decreases. Molecular dynamics out from the nematic layer is quite similar to that of the bulk.

R1.00288 ABSTRACT WITHDRAWN —

R1.00289 Electric Polarization and ME effect in layered iron oxide, SUMIO ISHIHARA, MAKOTO NAKA, JOYOI NASU, Department of Physics, Tohoku University — Rare-earth iron oxides $\text{R}Fe_{2}O_{4}$ (R: rare-earth elements) is an exotic dielectric material with charge-order driven electric polarization and magnetoelectric effect caused by spin-charge coupling. The crystal structure consists of paired Fe-O triangular lattices and $R$-O block ones alternately stacked. Since a nominal valence of Fe ion is 2.5+, an equal amount of $\text{Fe}^{2+}$ and $\text{Fe}^{3+}$ coexists in the paired triangular lattices. In the electron diffraction experiments, Bragg reflections at (h/3 h/3 m +1/2) appear below 320K($\equiv T_{C0}$) in $\text{LuFe}_{2}O_{4}$. This observation indicates a valence order of Fe ion, i.e. a charge order of the Fe $3d$ electrons. Around $T_{C0}$, a spontaneous electric polarization and dielectric anomalies turn up. Moreover, around the ferrimagnetic spin ordering temperature ($T_{C0} = 250K$), the gigantic ME effects are recently discovered. We present a theory of a dielectric magnet $\text{RFe}_{2}O_{4}$ as an electronic ferroelectric and multiferroic material [1]. We address the following issues: (i) origin of the electric polarization and the FE transition, (ii) mechanism of the coupling between electric polarization and magnetization. Present study shows that the novel dielectric properties in this material arises from interplay among the geometrical frustration and the multi-degrees of freedom of electron.


R1.00290 Fermi surface and local density of states of ordered and disordered stripes, MATS GRANATH, Goteborg University — For a doped antiferromagnet with short-range spin stripe correlations and long-range charge stripe order the manifestation of charge order changes abruptly as a function of momentum along the Fermi surface. The disorder averaged local density of states is isotropic when integrated only over states which contribute to the “antinodal” spectral weight. An effectively two dimensional nodal liquid can thus coexist with static charge stripes provided there is no static spin order. For commensurate spin and charge stripe ordered systems the Fermi surface consists of a nodal hole pocket and an open “stripe band” section. Due to the stripe order the relation between hole density and size of a pocket will be reduced compared to a paramagnet by a factor of two for even charge period and four for odd charge period and we find an estimated upper limit on the area fraction of a hole pocket of 1.6% for charge period four and 4% for charge period five. We also discuss why electron pockets are not expected for a stripe ordered system and show that the open Fermi surface section may be electron like with a negative Hall coefficient.

R1.00291 Modification of amorphous carbon film surfaces by thermal grafting of alkenes monolayer, HUSSEIN SABBAH, SOURAYA AABOULI-GIRARD, FRANCINE SOLAL, CHRISTIAN GODET, BRUNO FABRE, MARYLINE GUILLOUX-VIRY, ANDRE PERRIN, STEPHANIE DEPUTIER, PHYSIQUE DES ATOMES, LASERS, MOLECULES, SURFACES (PALMS, UMR 6627), UNIVERSITE RENNES 1 TEAM, SCIENCES CHIMIQUES DE RENNES (UMR 6226), UNIVERSITE DE RENNES 1 COLLABORATION — The integration of molecules and semi-conductors opens new possibilities for large area devices in the fields of biochemical sensors, molecular electronics. This work aims at improving the control of the surface of amorphous carbon thin films, in order to optimize molecular grafting processes and investigate the electronic properties of molecular assemblies. Robust devices are expected from this coherent grafting, through strong C-C interface bonds. A quantitative comparison of thermally assisted gas phase and liquid phase processes using linear alkenes has been performed using X-ray photoelectron spectroscopy (XPS). In order to understand the grafting mechanisms and the a-C surface reactivity towards alkenes at different temperatures (160 - 300 °C), surface coverage values are compared using a-C films, with different average C sp$^3$ / sp$^2$ hybridization, residual oxygen contamination, surface densities and surface energies, as obtained from XPS, grazing angle X-ray reflectivity and contact angle measurements.

R1.00292 Calculated Zhang-Rice Singlet Dispersion in Mott-Insulators, XIANGANG WAN, QUAN YIN, SERGEY SAVRASOV, University of California, Davis — Using a combination of local density functional theory and cluster exact diagonalization based dynamical mean field theory (LDA+DMFT), we calculated many body electronic structures of several Mott-insulating oxides including undoped prototype high Tc materials. The dispersions of the lowest occupied electronic states are associated with the Zhang-Rice singlets (ZRS) in cuprates, and with doublets, triplets, quartets and quintets in more general cases. The spectral weight of ZRS band decreases as it approaches the BZ center, as observed by many recent ARPES experiments. Our results are in good agreement with experiments.
R1.00293 Exploration of Strongly Coupled Plasma Dynamics and Equilibrium Using the Particle-in-Cell Methodology1, D.V. ROSE, D.R. WELCH, T.C. GENONI, Voss Scientific, T.A. MEHLHORN, R.B. CAMPBELL, Sandia National Laboratories — Particle-based numerical simulations are required to study the dynamics and evolution of inhomogeneous nonequilibrium multispecies strongly coupled plasmas. Molecular-dynamics (MD) and particle-in-cell (PIC) techniques have been compared previously [K. Y. Sanbonmatsu, et al., J. Phys. IV (France) 10, Pr5-259 (2000)], with the PIC methodology demonstrating the capability of improved accuracy over the MD simulations at high resolution. However, the PIC simulations were significantly slower, limiting their utility. Here we explore several schemes to improve the computational speed of such calculations including non-iterative, implicit EM field solvers and subgrid models. The simulations are compared directly with the results of Sanbonmatsu, et al., and a new theoretical analysis of the hypernetted chain model where all inter-species correlations are retained [V. Schowar, et al., Contrib. Plasma Phys. 47, 324 (2007)].

R1.00294 Ionic salt-bridge dependence of dimerization of the GCN4 Leucine zipper, YANXIN LIU, PREM CHAPACAIN, BERNARD GERSTMAAN, Department of Physics, Florida International University, University Park, Miami, FL 33199 — The role that ionic interactions, or salt-bridges, play in protein folding and dimerization is still controversial. We perform computational simulations on the GCN4 leucine zipper to investigate the effect of ionic interactions. A three dimensional lattice model incorporating a Monte Carlo Metropolis Algorithm is employed to simulate the dimerization process. Our results show that stronger ionic interactions result in more stable dimers, in agreement with experiments. Our simulations also show that increasing the strength of the ionic interactions does not lead to a monotonous increase in the speed of the dimerization process. We find an optimal intermediate ionic interaction strength at which the dimer is stable and the dimerization process proceeds at the maximum rate. We present quantitative results of dimerization rates, heat capacity, and free energy landscapes as a function of the ionic strength for the GCN4 leucine zipper.

R1.00295 Entanglement of Uniformly Accelerating Schrödinger, Dirac, and Scalar Particles, WAI LIM KU, MING CHUNG CHU, Department of Physics and Institute of Theoretical Physics, the Chinese University of Hong Kong — We study how the entanglement of an entangled pair of particles in two different modes is affected when one or both of the pair is uniformly accelerated, while the detector remains in an inertial frame. We find that the entanglement is unchanged if all degrees of freedom are considered. However, particle pairs are produced when a relativistic particle is accelerated, and more bipartite systems emerge. We identify the particle and antiparticle excitations in the asymptotic regions where there is no acceleration, which corresponds to detection by inertial detectors. We calculate the entanglements between particles/antiparticles in the two modes, and we find that the distribution of entanglements into the different biparticle systems varies as the acceleration. In particular, the entanglement of a pair of accelerating fermions is transferred preferentially to the produced antiparticles when the acceleration is large, and the entanglement transfer is complete when the acceleration approaches infinity. However, no such entanglement transfer to the antiparticles is observed for scalar particles.

R1.00296 Experimental observation of solitons propagating in a hydro-mechanical array of one-way coupled oscillators1, KELLY M. PATTON, JAMES GALLAGHER, JOHN F. LINDNER, The College of Wooster, Wooster OH 44691 — Arrays of two-way coupled oscillators are familiar and have been extensively studied. However, arrays of one-way coupled oscillators have been studied only in the last five years, mainly computationally and theoretically. One-way coupling seems impossible, because it appears to violate Newton’s third law (and energy conservation). However, we have constructed arrays of one-way coupled oscillators by enabling each oscillator to modify an external force that does work on a neighboring oscillator. We observe solitons propagating in our arrays and compare their behavior with computer simulations and theory.

R1.00297 Cyclotron radiation and emission in graphene, TAKAHIRO MORIMOTO, University of Tokyo, YASUHIRO HATSUGAI, University of Tsukuba, University of Tokyo, HIDEO AOKI, University of Tokyo — While the physics of “Massless Dirac” particles in graphene has been kicked off by the observation of an anomalous quantum Hall effect, interests begin to extend optical properties, which includes recent spectroscopy studies including the effect of disorder to show the following: (i) The unevenly spaced Landau levels do give rise to an interesting situation, As for the relaxation processes, which are examined with an extention of the treatment for ordinary quantum Hall systems, graphene’s peculiar cyclotron energy $\sqrt{\hbar/m_e}$ along with its 2D nature favor the cyclotron emission over other relaxation processes.

R1.00298 ABSTRACT WITHDRAWN —

R1.00299 Structural Phase Transitions induced by Compressive and Tensile Strains in Ordered Sc$_{0.5}$Ga$_{0.5}$N and Sc$_{0.5}$In$_{0.5}$N Alloys, AHMAD ALSAAD, AHMAD AHMAD, Department of Physics, Jordan University of Science & Technology (JUST), Irbid-22110, Jordan, CONDENSED MATTER GROUP TEAM — Local-density approximation calculations (LDA) within density functional theory (DFT), Berry phase approach within modern theory of polarization and phonon calculations within the density functional perturbation theory are performed to predict the existence of breaking-symmetry structural phase transitions in ordered Sc$_{0.5}$Ga$_{0.5}$N and Sc$_{0.5}$In$_{0.5}$N alloys. It has been demonstrated that the existence of strain-induced structural phase transition leads to optimized optical, electronic, acoustic, and piezoelectric properties of ordered Sc$_{0.5}$Ga$_{0.5}$N and Sc$_{0.5}$In$_{0.5}$N. In particular, it has been shown that ordered Sc$_{0.5}$Ga$_{0.5}$N and Sc$_{0.5}$In$_{0.5}$N alloys at fixed Ga, In and Sc compositions exhibit tremendous piezoelectric response (i.e., the e$_{ij}$ piezoelectric coefficient adopts a huge value as large as 8.3 C/m$^2$) as a function of the in-plane compressive and tensile strains. In addition, several optical, electric, acoustic anomalies are shown and discussed. We also reveal the reason behind, and consequences of, these unusual properties associated with the biaxial strain-induced structural phase transitions.

3This research was supported by NSF-DMR 0649112 and The College of Wooster.

R1.00300 Characterizing soliton behavior in noise-mediated one-way coupled oscillators, CHRIS-TINE E. WEIDERT, BARBARA J. BREEN, University of Portland, JOHN F. LINDNER, The College of Wooster — While arrays of coupled bistable oscillators have been extensively studied, the unique behavior of such arrays under one-way coupling has been studied only in the last few years. Using numerical simulations run on a high-speed parallel computing cluster and theoretical arguments, we show that the speed of solitons propagating in these arrays is proportional to the coupling strength. In addition, we refine and improve a metric, the complexity, that quantifies the intricacy of the spatiotemporal behavior of the array as a function of coupling and noise.
R1.00301 Wetting-like phase transitions in a surface-enhanced type-I superconductor

VLADIMIR KOZHEVINIKOV, Tulsa Community College, MARGRIET VAB BAEL, Katholieke Universiteit Leuven, Belgium, PRATAP SAHOO, Paul Scherrer Institut, Switzerland, KRISTIAAN TEMST, CHRIS VAN HAESENDONCK, ANDRE VANTOMME, JOSEPH INDEKEU, Katholieke Universiteit Leuven, Belgium — Superconductivity in single crystal Sn samples with surface enhanced order parameter was studied experimentally. Controllable surface enhancement was achieved by mechanical polishing or by ion irradiation. A first-order surface superconductivity transition was found in parallel magnetic fields close to the bulk critical field Hc(T) and for temperatures above 0.8Tc up till a surface critical temperature Tcs higher than Tc, where Tc is the bulk critical temperature. The resulting phase diagram agrees with that predicted for interface delocalization or wetting transitions in type-I superconductors, based on the Ginzburg–Landau theory.

1This research has been supported by the K U Leuven Research Council (F/05/049, GOA/2004/02 and INPAC EF/05/005), project G.0237.05 of the FWO Vlaanderen, and IUAP P5/1.

R1.00302 Viscoelastic Relaxation of Molten Phosphorus Pentoxide

DAVID SIDEBOTTOM, Creighton University, JESSICA CHANGSTROM — We report the first ever dynamic light scattering study of the viscoelastic relaxation in anhydrous liquid P2O5. Properties of the time decay of the dynamic structure factor, including the average structural relaxation time and the stretching exponent, were obtained for temperatures from 850 °C to near the glass transition (Tg = 419 °C) using photon correlation spectroscopy. Analysis indicates that P2O5 is a strong glassforming liquid but one which exhibits an abnormal non-exponential relaxation near Tg. The viscoelastic behavior of P2O5 is compared with that of its metaphosphate counterpart to demonstrate how changes in bond connectivity influence both fragility and levels of dynamic heterogeneity.

1The support of Petroleum Research Fund (Grant No. 43743-G110) is gratefully acknowledged.

R1.00303 Structural distortions in the spin-gap regime of the quantum antiferromagnet SrCu2(BO3)2

CARLO VECCHINI, IESL-FORTH, Heraklion, Greece, LAURENT CHAPON, ISIS Facility, STFC-RAL, Didcot,OX110QX, UK, HIROSHI KAGEYAMA, Chemistry Department, Kyoto University, Kyoto,606-8502, Japan, OTHON ADAMPOULOS, ALEXANDROS LAPPAS, IESL-FORTH, Heraklion, Greece — Since the so-called pseudo spin-gap was suggested to be relevant for the appearance of high-Tc superconductivity, a number of studies have been made on low-dimensional quantum spin systems with a singlet ground state. SrCu2(BO3)2 is an example of a 2D frustrated magnet in which a rectangular network of spin-1/2 Cu dimers displays a spin-gap (Tc<20K). Spin anisotropies are needed to describe accurately the dynamics of this 2D orthogonal dimer model. Accurate neutron lattice symmetry is necessary to rationalize the ground state properties. This is the first detailed crystallographic study within the gap region. Our powder neutron diffraction reveals distortions of the tetragonal structure that uncover an intimate spin-lattice coupling. The interdimer Cu-O-Cu angles increase abruptly by 0.4 deg, consistent with strengthening of the superexchange interaction. This is accompanied by a sharp reduction of the static buckling within the CuO2 planes and a contraction of the interlayer distances. We discuss the role of the structural deformations and the symmetry rules imposed for the development of the Dzyaloshinsky-Moriya exchange.

R1.00304 Hypervelocity Impact on Interfaces: A Molecular-Dynamics Simulations Study

MARTINA E. BACHLECHNER, Fairmont State University, ELI T. OWENS, ROBERT H. LEONARD, BRONWYN C. COCKBURN, West Virginia University — Silicon/silicon nitride interfaces are found in micro electronics and solar cells. In either application the mechanical integrity of the interface is of great importance. Molecular-dynamics simulations are performed to study the failure of interface materials under the influence of hypervelocity impact. Silicon nitride plates impacting on silicon/silicon nitride interfaces targets of different thicknesses result in structural phase transformation and delamination at the interface. Detailed analyses of atomic velocities, bond lengths, and bond angles are used to qualitatively examine the respective failure mechanisms.

1North Carolina State University

R1.00305 Nanoscale X-ray Diffraction Microscopy at the Nanoprobe Beamline

MARTIN HOLT, ROBERT WINARSKI, JORG MASER, X-ray Imaging Group, Center for Nanoscale Materials, Argonne National Laboratory — The near-term completion of the Nanoprobe Beamline at the Advanced Photon Source as part of the Center for Nanoscale Materials Project will provide a dedicated facility for hard X-ray microscopy at a 30 nm spatial resolution. Integrating a high-flux synchrotron X-ray beamline with an advanced optomechanical experimental platform at an energy range of 3-30keV will make possible nanoscale studies of functional and biological materials with a high degree of precision and efficiency. The unique capabilities of hard X-ray microscopy techniques such as large penetration depths, experimental sensitivity to elemental composition, crystallographic phase, and strain when applied at this length scale offer unique opportunities for many fields of sciences. The challenges and scientific impact of extending X-ray microscopy techniques such as scanning probe X-ray fluorescence, scanning probe microdiffraction, spectroscopy, tomography, and full-field imaging to the nanoscale will be discussed.

R1.00306 Hard X-ray Nanoprobe Development at Argonne National Laboratory

ROBERT WINARSKI, MARTIN HOLT, JORG MASER, VOLKER ROSE, DEMING SHU, BRIAN STEPHENSON, Argonne National Laboratory, CENTER FOR NANOSCALE MATERIALS / ADVANCED PHOTON SOURCE COLLABORATION — The HarX-ray Nanoprobe beamline will explore nanoscale objects at a spatial resolution of 30 nanometers, using x-ray fluorescence spectroscopy, transmission imaging, diffraction, and scattering. X-ray fluorescence measurements will provide element-specific imaging of individual nanoparticles inside of samples. Transmission imaging will allow three dimensional mappings of thick specimens and devices. X-ray diffraction and scattering capabilities will examine strain states and ordering in nanoscale systems. The beamline is designed for two modes of operation: a scanning probe mode, where the spatially coherent fraction of the x-ray beam is focused by high-resolution x-ray optics onto a small area of a sample, and a full-field transmission mode, where the full, partially coherent x-ray beam is used to illuminate a sample for transmission imaging at high resolution.

2This research, including use of the Center for Nanoscale Materials, was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357.

R1.00307 Low temperature growth of boron nitride nanotubes

CHEE HUEI LEE, MING XIE, JIESHENG WANG, YOKE KHIN YAP — Boron nitride nanotubes (BNNTs) are promising nanostuctures that will complement the applications of carbon nanotubes in various emerging areas. However, the synthesis of BNNTs is still challenging and required high growth temperatures (1500 °C to 3000 °C). Here we will discuss about two approaches for low temperature growth of BNNTs. First, we have reported on the growth of pure BNNTs at 600 °C by a plasma-enhanced pulsed-laser deposition (PE-PLD) technique [1]. These BNNTs were grown vertically-aligned on substrates. Latest result on the effect of catalyst, growth temperatures, ambient gas pressures, substrate bias voltages and the growth mechanism will be discussed in the meeting. Secondly, effective growth of BNNTs is recently achieved by conventional thermal chemical vapor deposition (CVD). Our new CVD approach leads to effective growth of long and clean BNNTs at 1200 °C. SEM, TEM, EELS, Raman, FTIR, and UV absorption data indicate that these BNNTs are having high structural ordered and a energy band gap > 5.6 eV. [1].


3Y.K.Yap acknowledges support from the National Science Foundation CAREER awards (Award No. 0447555, Division of Materials Research).
R1.00308 Non-affine deformations in biological gels, QI WEN, ANINDITA BASU, JESSAMINE WINNER, ARJUN YODH, PAUL JANMEY, University of Pennsylvania — Compared to flexible polymer gels, filamentous biopolymer networks generally have larger elastic moduli, a striking increase in elastic modulus with increasing strain, and a pronounced negative normal stress when deformed under simple shear. Different theoretical models based on either entropic elasticity of semiflexible filaments or enthalpic bending and stretching of rods can under some conditions account for all three of these unusual features. An essential difference between theories that relate microscopic structural parameters such as persistence length and mesh size of biopolymer gels to their macroscopic rheology are predictions about whether deformation of these materials is affine. We test the validity of this affine assumption by embedding micron-sized fluorescent beads within the networks and quantifying their displacements under shear deformation. Measures of non-affine deformation are small for networks of thin relatively flexible filaments and get smaller as strain increases. The small non-affine measures are consistent with the entropic model for non-linear elasticity of semiflexible polymer networks. However, as filament stiffness and mesh size increases the deformations become more non-affine, these results are more possible consistent with enthalpic bending and stretching models.

R1.00309 Interference in the Mott Insulator State of Distinguishable Particles, LIN TIAN, FUMITAKA FUJIWARA, TIM BYRNES, National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan, YOSHIHISA YAMAMOTO, Department of Applied Physics and E. L. Ginzton Laboratory, Stanford University, Stanford, CA 94305; National Institute of Informatics, Tokyo, Japan — Particle statistics plays a crucial role in strongly interacting quantum many-body systems. Here, we study the Hubbard model for distinguishable particles at unit filling. We show that when on-site repulsive interaction dominates over tunneling, the ground state is a Mott insulator state with higher order coherence between the particles. This result can be experimentally confirmed by the recovery of the interference pattern in the density correlation functions and is robust against non-uniformity of the interaction and tunneling parameters. We also show that this state is a maximally entangled state, in contrast to its bosonic counterpart. L. Tian, F. Fujiwara, T. Byrnes, and Y. Yamamoto, preprint, arXiv/0705.2023.

R1.00310 Spin-state polarons as a precursor to ferromagnetism and metallicity in hole-doped LaCoO\textsubscript{3}, A. PODLENSYAK, M. RUSSINA, Hahn-Meitner-Institut, Berlin, Germany, E. POMJAKUSHINA, K. CONDER, Paul Scherrer Institut, Switzerland, D. KHÖMISKII, Institute of Physics II, University of Cologne, Germany — Lightly doped cobaltites La\textsubscript{1-y}Sr\textsubscript{y}CoO\textsubscript{3} exhibit magnetic properties at low temperatures, in strong contrast to the diamagnetic LaCoO\textsubscript{3}. We undertook an inelastic neutron scattering study with the goal to identify the energy spectrum and magnetic state of cobalt ions in the doped system with x = 0.002. In distinguish to the parent compound, where no excitations have been found for T < 30 K, an inelastic peak at \Delta E \sim 0.75 meV was observed in La\textsubscript{0.998}Sr\textsubscript{0.002}CoO\textsubscript{3} at T = 1.5 K. The intensity of this excitation is much higher than what is expected from an estimated concentration of doped holes. Furthermore, strong Zeeman splitting of the inelastic peak corresponds to an unusually high effective magnetic moment \sim 15\mu_B. Neighboring low-spin (LS) Co\textsuperscript{3+} and intermediate-spin Co\textsuperscript{3+} ions can share an e\textsubscript{g} electron by swapping configuration. The two \textsubscript{t}_{2g} electrons, in their turn, couple ferromagnetically. Therefore, we propose that the holes introduced in the LS state of LaCoO\textsubscript{3} are extended over the neighboring Co sites forming spin-state polarons and transforming the involved Co\textsubscript{3+} to the higher spin state. Grows of spin-state polarons with hole doping finally results in a metallic ferromagnetic state for x > 0.3.

R1.00311 Metal-insulator transition in graphene oxide, GEUNSIK LEE, KYEONGJAE CHO, Department of Physics and Department of Electrical Engineering, University of Texas at Dallas, Texas 75080, USA — Using the first-principles density-functional theory method, we show that metallic graphene undergoes a metal-insulator transition upon adsorption of oxygen, and that the fully oxidized metastable graphene has a large energy gap of 3.27 eV. Graphene oxide (GO) shows the transition at the coverage of 1/3 - 1/2 monolayer of epoxide group. Each O atom saturates two \pi orbitals, and the GO band structure is determined by the connectivity of metallic channels of \pi orbitals. Although such directional conduction is verified for most of GOs that we considered, we have found that longer range interaction between \pi orbitals also plays an important role in the electronic structure of GOs. We apply our results to the implication on electrical conductions in dry and wet GO samples.

R1.00312 Tight-binding Calculation of Electronic Properties of Oligophenyl and Oligoacene Chains, ADAM HINKLE, ANTONIO C. CANCIO, MAHFUZA KHATUN, Ball State University — Within recent years, allotrophic structures of carbon have been produced in the forms of tubes and ribbons which offer the promise of extraordinary electronic and thermal properties. Here we present analyses of oligophenyl and oligoacene systems—finite, one-dimensional chains of benzene rings linked along the armchair and zigzag directions. These one-dimensional structures, which are amenable to calculation by analytical means, exhibit features very similar to carbon nanotubes and nanoribbons. Using a tight-binding Hamiltonian we analytically determine the energy bands of these systems. From these results we calculate the density of states and wavefunction symmetries for each structure. We also discuss the effect doping has on the energy as well as examine the transport properties.

R1.00313 Investigation of colloidal interactions in nanoparticle suspensions with a single optical trap, JOSEPH JUNIO, ERIC BLANTON, H. DANIEL OU-YANG, Lehigh University — Colloidal interaction parameters such as virial coefficients or bulk moduli are traditionally measured by scattering methods. However, experimental difficulties often limit the range of applications of these methods to idealized systems. Multiple optical tweezers have also been used to study interparticle forces, but this has been limited to micron size individual particles at infinite dilution. We propose a new approach to investigate many body deformations of sub-micron colloidal particles in native suspensions with a single optical trap. Using a blinking optical trap and confocal detection of optical signals, this approach can be used to measure many body interactions in suspensions of colloidal particles in the range of tens to hundreds nanometers in size. Theoretical calculation and preliminary experimental data will be presented at the talk.

R1.00314 3-D structure and dynamics of microtubule self-organization, JING WANG, H. DANIEL OU-YANG, Lehigh University — Laser scanning confocal microscopy was used to study the dynamics of 3D assemblies spontaneously formed in microtubule (MT) solutions. Microtubule solutions prepared by mixing and incubating tubulin in the presence of GTP and Oregon Green conjugated taxol in PM buffer were placed in long, sub-millimeter thin glass cells by the capillary action. Within 24 hours, starting with a uniform distribution, microtubules were found to be gradually separated into a few large “buckled” bundles along the long direction, and in the middle plane, of the sample cell. A well-defined wavelength of the buckling sinusoids along the short direction of the bundles was approximately 40 \mu m in diameter and the lengths were several centimeters. Detailed analysis of the 3-D image within the bundles revealed that each bundle seemed to consist of loosely packed MTs. It appeared that MTs were phase separated resulting from attractive interactions between charged MT fibers. The “buckling” behavior could be the result of geometrical constraints of the repulsive cell walls and the repulsive interaction between bundles. Detailed 3-D observations of the dynamic evolution of MT assembly could provide insight to the mechanisms of cellular MT organization and phase separation of charged colloidal rods.

1This work is supported in part by NSF-DMR 0421259

2This work is supported in part by NSF-DMR 0421259
R1.00315 Genetic Engineering of Optical Properties of Biomaterials\textsuperscript{1}, PAUL GOURLEY, Sandia Labs, ROBERT NAVIAUX, MICHAEL YAFFE, Univ. CA San Diego, SANDIA NATIONAL LABS COLLABORATION, U C SAN DIEGO COLLABORATION — Baker’s yeast cells are easily cultured and can be manipulated genetically to produce large numbers of bioparticles (cells and mitochondria) with controllable size and optical properties. We have recently employed nanoplasmonic spectroscopy to study the refractive index of individual cells and isolated mitochondria from two mutant strains. Results show that biomolecular changes induced by mutation can produce bioparticles with radical changes in refractive index. Wild-type mitochondria exhibit a distribution with a well-defined mean and small variance. In striking contrast, mitochondria from one mutant strain produced a histogram that is highly collapsed with a ten-fold decrease in the mean and standard deviation. In a second mutant strain we observed an opposite effect with the mean nearly unchanged but the variance increased nearly a thousand-fold. Both histograms could be self-consistently modeled with a single, log-normal distribution. The strains were further examined by 2-dimensional gel electrophoresis to measure changes in protein composition. All of these data show that genetic manipulation of cells represents a new approach to engineering optical properties of bioparticles.

\textsuperscript{1}Supported by DOE Office of Basic Energy Sciences

R1.00316 Ambient-pressure thermodynamic measurements on UGe\textsubscript{2}, F. HARDY, C. MEINGAST, H. VON LOEHNEYSEN, Forschungszentrum Karlsruhe, Institut fuer Festkoerperfysik,76021 Karlsruhe, Germany, Physikalisches Institut, Universitaet Karlsruhe, 76128 Karlsruhe, F. FLOQUET, A. HUXLEY, SPMS-DRFM, CEA/ Service de Recherche en Matiere Condensee, France, J. LASHLEY, Materials Science Division and Technology Division, LANL, Los Alamos, New Mexico 87545, USA, R.A. FISHER, N.E. PHILLIPS, Materials Science Division, LBNL, Berkeley, California 94720, USA. — The pairing interaction leading to the formation of the Cooper pairs remains unidentified in the ferromagnetic superconductor UGe\textsubscript{2}. Nevertheless, there is strong experimental evidence that superconductivity is not mediated by the magnetic fluctuations that drive T\textsubscript{Curie} (p) to zero; it rather appears closely related to another phase boundary T\textsubscript{p} (p) that occurs at lower pressure. Theoretical works suggested that this additional phase boundary could arise either from a coupling between SDW and CDW orderings or from a peak in the electronic density of states. Although the existence of this anomaly is experimentally incontestable between 0.6 and 1.2 GPa, the situation at ambient pressure remains ambiguous. We discuss the aforementioned scenario in the light of recent high-resolution thermal expansion and calorimetric measurements realized under high magnetic fields at ambient pressure.

R1.00317 Ressonance Raman Excitation Energy Map and High Resolution Transmission Electron Microscopy of hundreds of (n,m) Single Wall Carbon Nanotubes\textsuperscript{1}, ADO JORIO, PEDRO B.C. PESCE, PAULO T. ARAUJO, Universidade Federal de Minas Gerais, STEPHEN K. DOORN, Los Alamos National Laboratory, PASHA NIKOLAEV, ERC/NASA-JSC, UFMG COLLABORATION, NASA COLLABORATION, LANL COLLABORATION — In this work we measure the Raman spectra of a single wall carbon nanotube (SWNT) sample with a wide diameter distribution - 1nm to 6nm - with closely spaced laser lines over the 1.26eV to 2.71eV energy range and did a thorough analysis of the observed features. The most intense peaks are assigned to the scattering of light by a single RBM phonon in resonance with the well-known excitonic E\textsubscript{11} transitions. Comparison of the Raman map with the diameter distribution of the sample, obtained from high resolution transmission electron microscopy (HRTEM) measurements of 395 different nanotubes allows us to determine the diameter dependence of the RBM cross section. Furthermore, a number of weaker features are identified with different mechanisms, such as the RBM overtone and cross polarized transitions.

\textsuperscript{1}Support from CNPq, Brazil.

R1.00318 Ripples in epitaxial graphene, FRANCOIS VARCHON, PIERRE MALLET, JEAN-YVES VEUILLEN, LAURENCE MAGAUD, Institut Neel CNRS/UJF — On the basis of extensive ab initio calculation supported by scanning tunneling experiments, we have elucidated the complex morphology of the graphene/SiC (0001) interface \textsuperscript{1}. We demonstrate that a carbon buffer layer is always present at the interface. It is a key characteristic of the system because this buffer layer electronically decouples the graphene layer from the substrate \textsuperscript{2}. It has a mosaic structure that is reminiscent of a graphene honeycomb lattice distorted by the formation of strong covalent bonds with the substrate. The substrate-induced nanostructuration extends up to the ontop graphene layer where it generates an incommensurate modulation of the honeycomb lattice. The possible opening of a gap induced by the substrate \textsuperscript{3} in the epitaxial graphene electronic structure will also be discussed. \textsuperscript{1}F.Varchon et al. cond-mat/0712.3394, (submitted to PRB) \textsuperscript{2}F.Varchon et al. Phys. Rev. Lett. 99, 126805 (2007) \textsuperscript{3}S.Y.Zhou et al. Nature Mat. 6, 771 (2007)

R1.00319 Phase transition via intermediate state and control of piezoelectric parameters in lead-zirconate-titanate based solid solutions\textsuperscript{1}, V. SOBOLEV, South Dakota School of Mines & Technology, V. ISCHCHUK, Institute for Single Crystals, NAS of Ukraine, 61001 Kharkov, Ukraine, N. SPIRIDONOV, STC “Reaktivelektron”, NAS of Ukraine, 83096 Donetsk, Ukraine — Presentation contains results of experimental investigation of the influence of external electric field on the stability of phases in antiferroelectric substances with a small difference in the free energies of the ferroelectric and antiferroelectric states. The composition-electric-field phase diagrams with intermediate states of coexisting domains of the ferroelectric and antiferroelectric phases are obtained for lanthanum-modified lead-zirconate-titanate based solid solutions. This intermediate state appears in the process of inducing of the ferroelectric state by an external electric field in antiferroelectric solid solutions. Peculiarities of the intermediate state caused by interphase interactions between coexisting ferroelectric and antiferroelectric domains are revealed. Analysis of the dependences of piezoelectric material parameters on external electric field at the phase transition via an intermediate state has been performed. It is demonstrated that within the interval of existence of the intermediate state the piezoelectric material parameters can be effectively controlled by an applied electric field.

\textsuperscript{1}Partially supported through ONR Grant No. N00014-06-1-0616 and STCU Grant No. 3898.

R1.00320 Entangled Photon Quantum Key Distribution: Theory and Experiment, ISRAEL OWENS, Los Alamos National Laboratory — Secure communications face growing challenges due to technological advances such as the anticipated arrival of quantum computers. Quantum key distribution offers a new method for the distribution of cryptographic key material that is secure against these challenges. I will describe a method of quantum key distribution that is based on using entangled photon pairs (EQKD). In particular, I will discuss and emphasize the key theoretical and experimental components of EQKD and the details of recent test-bed data results.

R1.00321 Zero dimensional area law in a gapless fermion system\textsuperscript{1}, GREGORY LEVINE, DAVID MILLER, Hofstra University — The entanglement entropy of a gapless fermion subsystem coupled to a gapless bulk by a “weak link” is considered. It is demonstrated numerically that each independent weak link contributes an entropy proportional to ln L, where L is linear dimension of the subsystem.

\textsuperscript{1}Supported by an award from Research Corporation CC6535

R1.00322 E=2mc\textsuperscript{2}, KWADWO DOMPREH, University of Cape Coast — The Albert Einstein mass-energy equation E=mc\textsuperscript{2} which is used primarily in the estimation of the amount of energy in fission reaction can be modified to give an equation which is used calculate the amount of energy in a fusion reaction. This theory is deduced using the Gedenken experiment used in special relativity and a computer simulation using the Matrix laboratory. The energy harnessed is non — radioactive and can be used to power our homes, industries and even our automobiles. When the equation is applied to cosmological bodies such as the Suns, Starts and others gives a better understanding of their origin.
R1.00324 Ion Size Effect on Glow Peak Temperature in Dielectric Binary Mixed Crystals Doped With Divalent Europium, RICARDO RODRIGUEZ-MIJANGOS, RAUL PEREZ-SALAS, Universidad de Sonora — Thermoluminescence measurements at room temperature of “beta” irradiated divalent Europium doped binary mixed alkali halides with RbCl and KBr components at several concentrations x in molar fraction are carried out. The experiments have been carried out to identify the effect of composition in thermoluminescence glow peaks. A typical glow peak has been distinguished for each composition. A linear dependence of its temperature on the composition x has been found. This is principally associated with the radii size change of halogen ions. Comparison with results in mixed KCl:KBr, KBr:RbBr and KCl:RbCl support that assertion.

R1.00325 Consistent Hybrid Simulation of MD and CFD, SHUGO YASUDA, RYOICHI YAMAMOTO, Department of Chemical Engineering, Kyoto University; CREST, Japan Science and Technology Agency — The idea of multi-scale hybrid simulation is expected to be very useful for overcoming several difficult problems remain unsolved in frontiers of computational science in general. A striking example is the case of hydrodynamics of complex fluids or soft matters, for which neither reliable constitutive relation is known explicitly. Our strategy to overcome this problem is very straightforward. We are developing a multi-scale hybrid method which combines computational fluid dynamics (CFD) as a fluid solver and molecular dynamics (MD) as a direct generator of constitutive relations in a consistent way. The numerical algorithm is rather simple. We perform usual lattice-mesh based simulations for CFD level, but each lattice is associated with a small MD cell which generates a “local stress” according to a “local flow field” given from CFD instead of using any constitutive functions at CFD level. Some algorithms to smooth out noses arising from MD simulations in a consistent way are being developed. Comparisons of the numerical results obtained by our hybrid-simulations and those by normal CFDs with a Newtonian constitutive relation are made in order to show the validity of our hybrid simulation method.

R1.00326 Manipulation of the vibration of cold ground-state Cesium molecules, MATTHIEU VITEAU, AMODEN CHOTIA, MARIA ALLEGRINI, DANIEL COMPARAT, PIERRE PILLET, Laboratoire Aimé Cotton, CNRS, Université Paris-Sud, Bâtiment 505, Campus d’Orsay, 91405 Orsay, France — Creating in an efficient way, a large and dense sample of ultracold molecules in their fundamental ground state, i.e. with neither vibration nor rotation, is an important step toward the realization in further experiments. Among them, cold collisions, controlled chemistry, or accurate spectroscopic measurement. One further motivation is the possibility to go towards the realization of a Bose-Einstein molecular condensate. But all existing experiments of cold molecules (Feshbach resonance, photoassociation) formed molecules in high vibrational state, mostly close to the dissociation limit. We want to explore different schemes to create or transfer cold molecules (Cs2) to the electronic and vibrational fundamental state (Σv=0). We have studied the photoassociation of cold atoms in a high vibrational level (1Σg+ or 3Σg−) follow by an optical pumping scheme. We use a shaped femtosecond laser to realize the optical repumping step in order to excite the molecules to a potential which have good decay to lower vibrational levels.

R1.00327 Thermodynamically stable noncomposite vortices in mesoscopic two-gap superconductors, LIUVI CHIBOTARU, VU HUNG DAO, University of Leuven and INPAC — Two-gap (or two-band) superconductors such as recently discovered MgB2 show new qualitative effects with respect to conventional ones. For example the fractionalization of the magnetic flux associated to individual vortices is predicted in massive two-gap superconductors. It can either result from the inequality of the winding numbers of the vortices in the two condensates (L1 ≠ L2) having a common vortex core (composite vortices), or the vortex cores in each of the two bands can be spatially separated (noncomposite or deconfined vortices). In both cases they never correspond to the ground state, i.e. are thermodynamically unstable. Thus only the usual Abrikosov vortices are experimentally observed in massive two-gap superconductors. Within the two-gap Ginzburg-Landau theory we have found the existence of thermodynamically stable noncomposite vortices in mesoscopic superconductors in a large domain of the T − H phase diagram. The appearance of these vortex phases is caused by a non-negligible effect of the boundary of the sample on the superconducting order parameter and represents therefore a genuine mesoscopic effect. For low values of interband Josephson coupling vortex patterns with L1 ≠ L2 can arise in addition to the phases with L1 = L2. The calculations show that noncomposite vortices could be observed in thin mesoscopic samples of MgB2.

R1.00328 Destruction of global coherence in long superconducting nanocylinders, VU HUNG DAO, LIUVI CHIBOTARU, University of Leuven and INPAC — Recent realizations of the Little-Parks experiment on long hollow cylinders with nanoscale diameter have shown the destruction of superconductivity at zero temperature around half quanta of applied magnetic flux. In addition the observed resistive transition unexpectedely broadens when departing from zero magnetic field. A quantum phase transition near half flux quanta has been argued to explain this anomalous behavior. However this theory does not explain the step-like features observed in the temperature variation of the resistance. We show here that the puzzling behavior of the resistance results from an alternation of normal and superconducting sections along the tube. First within the Ginzburg-Landau theory we have found that the transition is of second order if the studied cylinders are homogeneous, which precludes the existence of nonhomogeneous phases. From this we conclude that phase separation must be triggered by the tube inhomogeneities. Within a minimal model where cylinder properties vary along its axis, our BCS calculations of the superconducting state are in a good agreement with experimental data, in particular, the multistep transitions are naturally explained. A small discrepancy near half flux quanta may be ascribed to the charge imbalance induced by the normal electron flow.

R1.00329 Long Time Tail of the Velocity Autocorrelation Function in a Two-Dimensional Moderately Dense Hard Disk Fluid, MASAHARU ISobe, Nagoya Institute of Technology — Alder and Wainwright discovered the slow power decay 1/√t (d/dimension) of the velocity autocorrelation function in moderately dense hard sphere fluids using the event-driven molecular dynamics simulations. In the two-dimensional case, the diffusion coefficient derived using the time correlation expression in linear response theory shows logarithmic divergence, which is called the “2D long- time tail problem”. We revisited this problem to perform a large-scale, long-time simulation with one million hard disks using a modern efficient algorithm and found that the decay of the long tail in moderately dense fluids is slightly faster than the power decay (∼ 1/t). We also compared our numerical data with the prediction of the self-consistent mode-coupling theory in the long time limit (∼ 1/(tv/vT)).
R1.00330 First and second order coherence of exciton-polariton condensates, G. ROUMPOS, C.W. LAI, E.L. Ginztun Lab., Stanford University, USA, A. FORCHEL, Technische Physik, Universität Würzburg, Germany, Y. YAMAMOTO, E.L. Ginztun Lab., Stanford University, USA — The microcavity exciton-polariton system offers the possibility to study condensed matter physics with optical techniques. In particular, condensation of microcavity exciton-polaritons in momentum space, as well as spontaneous buildup of spatial and temporal coherence, were recently demonstrated. We investigate the first and second order coherence of exciton-polariton condensates both in coordinate and in momentum space. We measured the spatial coherence length of up to 20 \( \mu m \), while \( g^{(2)}(t = 0) \) was measured to be close to 2 for appropriate near- and far-field filtering. This experiment provides insights into the phase and intensity fluctuations induced by polariton interactions.

1 Also in National Institute of Informatics, Japan
2 Also in National Institute of Informatics, Japan and NTT Basic Research Laboratories, Japan

R1.00331 Effect of terminal functional group of self-assembled monolayers formed on gold surface on the adsorption of Amyroid fibrils by AFM, KOHEI UOSAKI, MASAYA TSUKAMOTO, KAZUYASU SAKAGUCHI, YUYA ASANOMI, Hokkaido University — Amyroid fibril, which is known to cause BSE and Alzheimer disease, is a solid and stable fiber of several tens of nm wide and several \( \mu m \) long and has a potential to be used as nano-materials because functional molecules and metal and semiconductor nano-particles can be attached. However, it is not yet possible to align the Amyroid fibrils on a solid surface as programmed. In this study, interaction between Amyroid fibrils and self-assembled monolayers (SAMs) with various functional groups constructed on a gold surface was investigated by in situ AFM. Amyroid fibril (Aβ1-35) peptide was synthesized and the peptide was incubated at 37 deg. for more than a week to obtain the fibril. SAMs of alkyliols with methyl, OH, COOH, NH2, and SO3 groups were formed on Au(111) surface and AFM images were obtained by MAC mode in a solution containing the fibrils. It was clarified that electrostatic and hydrophobic interactions play important roles in adsorption behavior of the fibrils.

This work was supported by MEXT, Japan for Promotion of Novel Interdisciplinary Fields

R1.00332 Effect of nickel doping on the magneto-transport properties of Sm\( _{0.55} \)Sr\( _{0.45} \)MnO\( _3 \) manganites, MAHER ABDELHADI, University of Hail — We studied the effects of nickel (Ni) doping on the magneto-transport properties of Sm\( _{0.55} \)Sr\( _{0.45} \)MnO\(_3 \) manganites near the metal-insulator transition. Various concentrations of Ni-doped Sm\( _{0.55} \)Sr\( _{0.45} \)MnO\(_3 \) samples up to 5% were prepared (Ni was partially substituted at the Mn-site). The temperature dependence of resistivity and magnetoresistance were measured as a function of Ni concentrations. We observed a nonlinear reduction of the metal-insulator transition temperature (MIT) and a decrease in the width of the peaks in the temperature dependence of resistivity with increasing concentration of Ni. The peaks become sharper at high Ni concentration. The resistivity peaks at various magnetic fields collapses on themselves at the high temperature ends above the MIT.

R1.00333 Biomimetic nucleation of calcium carbonate layers at the air-water interface, KYUNGIL KIM, Northwestern University — The interaction between calcium carbonate crystals and chitosan at the air-water interface was investigated. Chitosan was selected as an organic, pseudo-structural component of calcium carbonate biominerals in the subphase in the presence of octadecyl sulfate Langmuir monolayers. Calcite crystallization was studied using X-ray diffraction and optical microscope techniques; in-situ grazing incidence x-ray diffraction was performed at synchrotron sources. Calcite crystallization under octadecyl sulfate monolayers shows a superlattice structure. This chitosan system also results in ACC (amorphous calcium carbonate) formation in the early stage of crystallization.

R1.00334 1H-NMR Study of Silica-Poly(epsilon-carbobenzyloxy-L-lysine) Composite Particles as Function of Temperature, ERICK SOTO, JEROME KOCH, DALE TRELEAVEN, PAUL RUSSO, Louisiana State University — Nearly monodisperse silica-poly(epsilon-carbobenzyloxy-L-lysine) composite particles were synthesized. The hydrodynamic radius of the composite particles and silica core was 200 and 100 nm respectively. Separately, poly(epsilon-carbobenzyloxy-L-lysine) was synthesized having a molecular mass of 200 kDa and a polydispersity of about 1.08. 1H-NMR spectra of the untethered polypeptide dissolved in deuterated m-cresol was collected at different temperatures ranging from 15 to 40 °C. The sharp change in the chemical shift of several protons at around 27 °C suggests a coil-helix conformation transition. Similarly, 1H-NMR spectra of the composite particles exhibits a more subtle change in chemical shifts in the explored temperature range suggesting a conformation transition of the tethered polypeptide.

1 This work was supported by NSF

R1.00335 An improved algorithm for the functional renormalization group and its application to two-dimensional Hubbard model, HIROKAZU TAKASHIMA, University of Tokyo, RYOTARO ARITA, Riken, KAZUHIKO KUROKI, University of Electro-Communications, Hideo Aoki, University of Tokyo, Rikun, KAZUHIKO KUROKI, University of Electro-Communications, Hideo Aoki, University of Tokyo — Among the methods that treat strongly correlated electron systems, the functional renormalization group (fRG) method has desirable a feature that it can take account of the shape of the Fermi surface with an unbiased inclusion of diagrams up to the one-loop level. Specifically, the temperature-flow functional renormalization group (T-flow fRG), proposed by Honerkamp and Salmhofer[1], can be a powerful method. We adopted the equal interval patch discretization in the Cartesian coordinates, for which we have constructed a fast and stable algorithm. With the present algorithm we discuss spin, charge, and pairing susceptibilities and the spectral function at low T for the two-dimensional Hubbard model, including the effect of t' and t". [1] C. Honerkamp and M. Salmhofer, Phys. Rev. B 64, 184516 (2001).

R1.00336 Dynamic nuclear polarization in biased quantum wires using spin-orbit coupling, VIKRAM TRIPATHI, Tata Institute of Fundamental Research, Mumbai, ANSON C. H. CHEUNG, NIGEL R. COOPER, University of Cambridge, Cambridge, United Kingdom — We propose a new method for dynamic nuclear polarization in a quasi one-dimensional quantum wire utilising the spin-orbit interaction, the hyperfine interaction, and a finite source-drain potential difference. In contrast with current methods, our scheme does not rely on external magnetic or optical sources which makes local control much more feasible. Using this method, a significant polarisation of a few per cent is possible in currently available InAs wires which may be detected by conductance measurements. This may prove useful for nuclear magnetic resonance studies in nanoscale systems as well as in spin-based devices where external magnetic and optical sources will not be suitable.

1 Supported by TIFR, Mumbai, Trinity College, Cambridge, and EPSRC
R1.00337 Storage capacity and retrieval time of small-world neural networks. HIRAKU OISHIMA, TAKASHI ODAGAKI. Department of Physics, Kyushu University — To understand the influence of structure on the function of neural networks, we study the storage capacity and the retrieval time of Hopfield-type neural networks for four network structures: regular, small world, random networks generated by the Watts-Strogatz (WS) model, and the same network as the neural network of the nematode Caenorhabditis elegans. Using computer simulations, we find that (1) as the randomness of network is increased, its storage capacity is enhanced; (2) the retrieval time of WS networks does not depend on the network structure, but the retrieval time of C. elegans's neural network is longer than that of WS networks; (3) the storage capacity of the C. elegans network is smaller than that of networks generated by the WS model, though the neural network of C. elegans is considered to be a small-world network. Reference: H. Oshima and T. Odagaki, Phys. Rev. E 76, 036114 (2007).

R1.00338 Current-Induced Magnetic Domain Wall Motion at Low Current Density via Perpendicular Anisotropy. SOON-WOOK JUNG, POSTECH, WOOJIN KIM, TAEK-DONG LEE, KAIST, KYUNG-JIN LEE, Korea University, HYUN-WOO LEE, POSTECH — The current-induced motion of magnetic domain walls carries great potentials for applications such as nano-scaled logic and memory devices. To achieve this goal, a large reduction in the threshold current density Jth for the domain wall motion is highly desired. Here we show that by introducing and properly exploiting the perpendicular magnetic anisotropy, Jth can be reduced by one or even two orders of magnitude in experimentally accessible parameter regimes. Using the collective coordinate approach, we analyzed the physical origin of the reduction. The analytic result was also tested by micromagnetic simulations of the LLG equation with spin transfer torque terms. The resulting Jth is insensitive to domain wall pinning forces and also to the non-adiabaticity, both of which are hard to control in experiments.

R1.00339 Probing Micromechanical Properties of Biological Cells by Oscillatory Optical Tweezers1. ANGELA ZAORSKI, Lehigh University, MING-TZO WEI, National Yang-Ming University, Taipei, Taiwan, HUSEYN C. YALCIN, JING WANG, SAMIR N. GHADIALI, Lehigh University, ARTHUR CHIOU, National Yang-Ming University, Taipei, Taiwan, H. DANIEL OU-YANG, Lehigh University — We used oscillatory optical tweezers to probe the micromechanical properties of cultured alveolar epithelial cells in vitro. The frequency-dependent viscoelasticity of these cells was measured by optical trapping and forced oscillation of either a submicron endogenous intracellular organelle (intra-cellular) or a 1.5μm silica bead attached to the cytoskeleton through trans-membrane integrin receptors (extra-cellular). Both the storage modulus and the magnitude of the complex shear modulus followed weak power-law dependencies with frequency. These data are comparable to data obtained by other measurement techniques. The exponents of power-law dependencies of the data from the intra- and extra-cellular measurements are similar, whereas, the differences in the magnitudes of the moduli from the two measurements are statistically significant.

R1.00340 Molecular magnetic coupling at atomic scale. JINFENG JIA, Department of Physics, Tsinghua University, Beijing 100084, China, YINGSHUANG FU, SHUAIHUA JI, Institute of Physics, The Chinese Academy of Sciences, Beijing 100080, China, XI CHEN, Department of Physics, Tsinghua University, Beijing 100084, China, XUCUN MA, Institute of Physics, The Chinese Academy of Sciences, Beijing 100080, China, QIKUN XUE, Department of Physics, Tsinghua University, Beijing 100084, China — Understanding and manipulating magnetic interactions between molecules is not only meaningful to molecular electronics, but also expected to have profound impact on the development of molecular spintronics and quantum computation. Tunneling spectroscopy of CoPc multilayer prepared on nanometer-sized Pb islands on Si(111) were measured with a subkelvin temperature scanning tunneling microscope. We observed magnetic excitations of coupled molecular systems via inelastic electron tunneling microscopy, and determined the coupling strength between CoPc adjacent layers with Heisenberg model. We further demonstrate the coupling between molecules, and coupling of single-molecule spin with metallic host can both be manipulated by changing their stacking sequence via molecular manipulation.

R1.00341 Model of the magnetostrictic motion of planar domain walls in ferromagnets and antiferromagnets1. MIKHAIL INDENBOM, JIAN-JUN LI, Laboratory of magnetism of Brittany CNRS, Brest, France — Recently we have shown that all details of magnetisation of magnetic thin films and multilayers deployed onto thin substrates can be revealed by simultaneous measurements of the substrate flexion and torsion. This technique is complimentary to the ordinary vector magnetometer being capable to resolve the signal from a ferromagnetic (F) layer with the magnetisation negligible compared to one of the other layers or even from an antiferromagnetic (AF) layer and to study, for example, the formation of planar domain walls in a spring-magnet F/F bilayer or an exchange-bias F/AF bilayer. In the current presentation we are using a 1D model of the planar domain wall in order to demonstrate a variety of magnetostrictive signals which can be obtained in such systems. For clarity we neglect the thickness, magnetic anisotropy and magnetostriction of the control F layer (an ideal F-layer). We have calculated how spin rotation induced in this layer by the applied magnetic field penetrates into the magnetostrictive AF or F layer and forms the planar domain wall.

R1.00342 Heat Transport in Epoxy Networks: A Molecular Dynamics Study. VIKAS VARSHNEY, Universal Technology Corporation, Dayton OH, SOUMYA PATNAIK, BARRY FARMER, AJIT ROY, AFRL, Wright Patterson Air Force Base, OH — In this poster, thermal behavior of a crosslinked epoxy network along with its un-crosslinked counterpart is presented using atomistic molecular dynamics simulations. The simulations were performed on EPON-862 and curing agent-W (DETDA), used as a model system using consistent valence force field (CVFF). The thermal transport is discussed in terms of its thermal conductivity, as calculated using both equilibrium as well as non-equilibrium molecular dynamics approaches, based on Green-Kubo and Fourier law formalisms, respectively. The results are found to be in good agreement with respect to experimental findings. Different energetic contributions of heat flux towards thermal conductivity and their possible coupling in terms of kinetic energy, van der Waals and electrostatic interactions are also discussed. In addition, the broad distribution of low frequency vibrational modes from power spectrum of velocity autocorrelation function suggests their disordered and amorphous nature. The poster also presents heat movement across a crosslinked slab using thermal relaxation simulations and estimates the thermal diffusivity, thermal relaxation time and mean free path for epoxy networks.

R1.00343 Electron Spin Resonance Force Microscopy of Spin Probes. ERIC W. MOORE, SANGGAP LEE, STEVEN A. HICKMAN, SEPPE KUEHN, JOHN A. MAROHN, Cornell University — Nitroxide spin labels, such as 4-amino TEMPO can be used to probe environmentally, conformal and structural probes in biological and polymer systems. We report on our efforts to detect electron spin resonance of 4-amino TEMPO in a polymer matrix using the magnetic resonance force microscopy as a proof of concept for future experiments on spin labeled proteins. Our microscope operates at high vacuum and low temperature, using a custom fabricated single crystal silicon cantilever in the magneto-cantilever geometry. The applied field is provided by a microstripline resonator at 18 GHz.

R1.00344 Electrical Transport in Ultra Long Bundles of Carbon Nanotube. AMELIA CHURCH, RAKESH SHAH, XIANFENG ZHANG, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale. We will present electrical transport measurements performed on bundles of millimeter long multi walled carbon nanotubes (MWNT). These MWNTs were grown using air assisted floating catalyst chemical vapor deposition method. The temperature dependence of resistance of these MWNT bundles as a function of bundle length will be presented. The variation in the electrical transport properties as a function of MWNT lengths as seen from the current-voltage measurements will also be discussed.
R1.00345 Benzene confinement in single-walled carbon nanotubes: inelastic and quasielastic neutron scattering , N.R. DE SOUZA, A.I. KOLESNIKOV, N. VERDAL, Argonne National Laboratory, Intense Pulsed Neutron Source, A.P. MORAVSKY, MER Corporation — We characterize experimentally the dynamic properties of benzene confined in single-walled carbon nanotubes (SWNT) of diameter 14 Å. The presence of benzene inside the nanotubes is demonstrated by measuring the small-angle neutron scattering intensities from a properly prepared C6D6 benzene — SWNT sample. The incoherent inelastic neutron scattering spectra from C6D6 benzene in the nanotubes and in the bulk crystal are measured at 4 K, up to an energy transfer of 130 meV. The effective vibrational density of states reveals a significant redistribution of all intermolecular modes for the confined benzene, whereas the intramolecular modes are nearly unaffected. Incoherent quasielastic neutron scattering spectra from C6D6 benzene in the nanotubes were also collected from 9 K to room temperature, at an energy-transfer resolution of approx. 80μeV. The orientational and translational diffusive dynamics of confined benzene are discussed on the basis of these data.

R1.00346 Patterned nanoring magnetic tunnel junctions and current-induced magnetization switching , Z.C. WEN, H.X. WEI, Y.N. HAN, X.F. HAN, Institute of Physics, CAS — Patterned nanoring (NR) magnetic-tunnel-junctions (MTJs) with outer diameters between 100 and 400nm and narrow ring widths between 25 and 30nm were successfully fabricated. The NR structure consists of CoFeB electrodes and Al-oxide barrier. The tunnelling magnetoresistance (TMR) ratio of the patterned NR-MTJs is in the range of 20%-50% observed at room temperature with \( R_A \) lower than 500Ωμm². These NR- MTJs allow current-induced magnetization switching with a low switching current density of around \( 9 \times 10^4 A/cm^2 \). Due to the small stray field and high TMR ratio, NR-MTJs offer superior prospects for high density magnetic random access memory (MRAM), recording medium and other spintronics devices.

R1.00347 Spin waves in 2D classical XY-model , SNEHADRI OTA, Institute of Physics, Bhubaneswar, SMITA OTA, Institute of Mathematics and Applications, Bhubaneswar — The description of phase transition in the microcanonical formalism has gained growing interest in recent years for the calculation of thermostatic properties of physical systems and microcanonical entropy.\(^1\) We have carried out micro-canonical Monte Carlo simulations of the 2D XY-model using periodic boundary conditions.\(^2\) In case of microcanonical Monte Carlo simulation some thermodynamic-like relations apply that allow definition of variable by averaging, specifically, the temperature. The energy distributions of the spins have been obtained for the the Kosterlitz-Thouless situation.\(^3\) In this case, the energy distribution of vortices show features that is due to spin waves, which agrees with the spin wave theory which predicts that \( E_{vortex} = -2 + T/2 \). References: \(^1\) H.Behringer and M.Pleimling, Phys.Rev.E 74 (2006) 11108 \(^2\) M.Creutz, Phys.Rev.Lett. 50 (1983) 1411 \(^3\) S Ota and S B Ota, Phys.Lett.A 367 (2007) 35 \(^4\) J B Kagot, Rev.Mod.Phys. 51 (1979) 659


R1.00349 Fabrication and characterization of InAs/AlGaSb HEMTs with high-k gate insulators , TOSHIHIKO MAEMOTO, KENJI FUJIWARA, TATSUYA INOUE, NAOKI AMANO, MASATOSHI KOYAMA, SHIGEHIKO SASA, MASATAKA INOUE, OSAKA INSTITUTE OF TECHNOLOGY TEAM — We report on the fabrication and characterization of InAs/AlGaSb high electron mobility transistors (HEMTs) with high-k gate insulators (Al₂O₃ and HfO₂). InAs/AlGaSb quantum well structures were grown by molecular beam epitaxy on a semi-insulating GaAs substrate [1]. From Hall measurements at room temperature, the as-grown wafer showed an electron mobility of 20,000-25,000 cm²/Vs and a sheet carrier density of 1.0-2.0×10¹² cm⁻². InAs/AlGaSb HEMTs have demonstrated a maximum extrinsic transconductance of 181mS/mm at room temperature. The gate leakage current has been markedly decreased by using thin high-k gate insulators. A typical gate current density of less than 1 nA/mm at room temperature was measured at 4 K, up to an energy transfer of 130 meV. The effective vibrational density of states reveals a significant redistribution of all intermolecular modes for the confined benzene, whereas the intramolecular modes are nearly unaffected. Incoherent quasielastic neutron scattering spectra from C6D6 benzene in the nanotubes were also collected from 9 K to room temperature, at an energy-transfer resolution of approx. 80μeV. The orientational and translational diffusive dynamics of confined benzene are discussed on the basis of these data.

R1.00350 Phonon Transport in Carbon Nanotubes , G. PENNINGTON, S.J. KILPATRICK, A.E. WICKENDEN, Army Research Laboratory — An understanding of phonon transport in carbon nanotubes (CNTs) is important considering potential electronic and thermal management applications. Weak intrinsic phonon scattering in these quasi-one-dimensional materials allows unique properties including high thermal conductivity. Thus CNTs may provide novel thermal management solutions critical for many emerging electronics technologies, including the development of high-power, high-temperature transistors/lasers and the continued scaling down of feature sizes in high-performance microelectronics. Carbon nanotubes are also expected to exhibit relatively large optical phonon decay times. It is widely believed that non-equilibrium phonons lead to conductance degradation, negative differential conductance, and enhanced thermal breakdown of suspended CNTs.\(^1\) Furthermore, absorption of hot optical phonons by conducting carriers would significantly alter device characteristics in the low-field ballistic limit. Thermal properties are also affected as the slow decay of hot optical phonons is expected to lead to reduced thermal diffusivity, and the development of inhomogeneous heating within a nanotube. In this talk, we discuss simulations of CNT phonon transport based on Monte Carlo solution of the phonon Boltzmann transport equation.\(^1\) References: \(^1\) E. Pop, D. Mann, J. Cao, Q. Wang, K. Goodson, and H. Dai, “Negative Differential Conductance and Hot Phonons in Suspended Nanotube Molecular Wires,” Phys. Rev. Lett., vol. 95, pp. 155505-8, October 2005.

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S1 DCMP: Diamond-based Quantum Information Processing Morial Convention Center
LaLouisiane AB
2:30PM S1.00001 Coherent control of single spins in diamond1. RONALD HANSON, Kavli Institute of Nanoscience Delft — Diamond-based materials have recently emerged as a unique platform for quantum science and engineering. Spins of single Nitrogen-Vacancy (N-V) color centers in diamond can be imaged, initialized and read out optically. These N-V center spins may allow for quantum information processing at room temperature, as measurements have shown long room-temperature electron spin coherence times well into the microsecond regime. We have investigated single N-V center spins that are coupled to electron spins of nearby nitrogen (N) defects, using magneto- optical imaging and coherent single-spin control at room temperature. Some of the N-V centers are strongly coupled to only one single N spin, allowing the controlled polarization and readout of this single ‘dark’ N spin. In contrast, other N-V centers couple to many N spins. We use these latter systems to study the canonical decoherence model of a single central spin coupled to a spin bath. By tuning the internal bath dynamics as well as the spin-bath coupling, we gain access to regimes with strikingly different behaviour. Finally, we have fabricated and characterized photonoc crystal microcavities in poly-crystalline diamond and observed quality factors up to 600. These structures are a first step towards controllable coupling of single N-V spins to single photons in a cavity-QED system in diamond.

1in collaboration with V.V. Dobrovitski, A.E. Feiguin, O. Gywat, C.F. Wang, E. Hu, and D.D. Awschalom. Financially supported by FOM, AFOSR and DARPA/CNID.


3:06PM S1.00002 Controlling individual electron and nuclear spins in diamond: from quantum registers to applications, MIKHAIL LUKIN, Harvard University — We will discuss our recent work involving the controlled manipulation of individual electron and nuclear spins in a high-purity diamond lattice. Our approach combines ideas from single molecule spectroscopy, quantum optical control techniques and the physics of mesoscopic spin ensembles. It allows us to isolate, polarize and manipulate single nuclear spins and use them to create quantum memory and small quantum registers. We will also describe novel applications of these techniques, including new approaches to quantum communication and computation as well as new quantum magnetic sensors with nanoscale resolution. Recent progress towards realization of these ideas will be discussed.

3:42PM S1.00003 Fabrication Strategies for Practical Diamond Based Quantum Information Processing Devices, STEVEN PRAWER, Centre of Excellence for Quantum Computer Technology and Quantum Communications Victoria, School of Physics, University of Melbourne, Australia — Optically emitting defect centres in diamond display a range of unique quantum properties that offer exciting possibilities for the construction of quantum devices which employ optical single-spin read-out. Indeed diamond is an ideal material for use in the fabrication of (i) single photon sources for quantum communications, (ii) optical fibre-based single spin read out systems, (iii) photonic platforms for the investigation of quantum entanglement in solid state systems and (iv) optical regenerators and non-linear quantum gates. The toolkit of available fabrication strategies which are used to engineer devices taking advantage of these unique properties will be presented. Our most recent results include demonstrations of (i) optical fibre based single photon sources based on Nickel and Nitrogen optical centres, (ii) waveguiding of light in structures hewn from single crystal diamond, (iii) Electrical Stark shift of the frequency of single optical emitters, (iv) coupling between the spins between single NV and N atoms in devices engineered by ion implantation, and (v) electromagnetically induced transparency in single NV centers. These crucial demonstrations establish the feasibility of a defect tolerant architecture for the fabrication of a few (~10-50) qubit diamond based quantum information processor. We will present one such possible architecture and explain the specific role for ion beam processing in the creation of qubits and the engineering of diamond photonic devices.

4:18PM S1.00004 Coherent Population Trapping of Single Spins in Diamond under Optical Excitation, CHARLES SANTORI, Hewlett-Packard Laboratories, Palo Alto, CA — The nitrogen-vacancy (N-V) center in diamond has long-lived electronic and nuclear spin coherence combined with optical addressability, making it an attractive candidate system for building a photonic network for quantum information applications. However, realizing such schemes will require control over the N-V energy level structure and integration into high-quality microphotonic structures operating at visible wavelengths. In this talk I will describe experiments on optical manipulation of N-V centers in low-nitrogen diamond samples. Typically the optical transitions of NV− are spin-conserving, so that if the N-V begins in the mS = 0 ground state, it can undergo many optical transitions before transitioning to mS = ±1. However, by applying stress to the crystal, or by using strain already present, it is possible to realize a Λ-type system with one excited state coupled by optical transitions to multiple ground states. By this technique we have observed coherent population trapping both in N-V ensembles and in single N-V centers. These results demonstrate the potential for all-optical spin manipulation in this system. I will also describe initial work on coupling N-V centers to photonic structures with the goal of enhancing emission into the zero-phonon line, as needed for applications such as quantum repeaters.

4:54PM S1.00005 Controlling single defects: Electric and magnetic fields, JOERG WRACHTRUP, Stuttgart University — Controlling the optical properties of single defects, e.g. its transition frequency and transition properties is an important prerequisite for their broad application. It is shown that external electric and magnetic fields allow for control over a broad range of parameters. The optical transition frequency can e.g. be controlled by an electric field. The same field determines whether the defect is driven cyclic or lambda transition behaviour dominates. The talk will describe current knowledge of the defect in this respect and show perspectives toward cavity coupling and entanglement of distant defects.

Wednesday, March 12, 2008 2:30PM - 5:30PM —
Session S2 FLAP: Can Power Dissipation in a Switch Be Significantly Lowered?
Morial Convention Center LaLouisiane C

2:30PM S2.00001 Will a New Milli-Volt Switch Replace the Transistor for Digital Applications? , ELI YABLONOVITCH, EECS Dept., University of California, Berkeley — In contemplating the headlong rush toward miniaturization represented by Moore’s Law, it is tempting to think only of the progression toward molecular sized components. There is a second aspect of Moores Law, that is sometimes overlooked. Because of miniaturization, the energy efficiency of information processing steadily improves. We anticipate that the energy required to process a single bit of information will eventually become as tiny as 1 electron Volt per function, truly a molecular sized energy. Inevitably most logic functions including storage, readout, and other logical manipulations will eventually be that efficient. However there is one information-processing function that bucks this trend. That is communication, especially over short distances. Our best projections of improvements in the short distance communication function show that it will still require hundreds of thousand of electron Volts, just to move one bit of information the tiny distance of only 10 micro meters. Why this energy per bit discrepancy for communications? It is caused by the difference in voltage scale between the wires and the transistor switches. Transistors are thermally activated, leading to a characteristic voltage $kT/q$. Wires are long and they have a low impedance, allowing them to operate efficiently even at 1-milli-Volt. The challenge then is to replace transistors with a new low-voltage switch, that is better matched to the wires. I will present some of the technical options for such a new switch.

3:06PM S2.00002 Use of negative capacitance to provide voltage amplification for ultra low power nanoscale devices, SAYEEF SALAHUDDIN, Purdue University — It is well known that conventional Field Effect Transistors (FET’s) require a change in the channel potential of at least 60 mV at 300K to effect a change in the current by a factor of ten, and this minimum subthreshold slope $S$ puts a fundamental lower limit on the operating voltage and hence the power dissipation in standard FET based switches. Here we show that by replacing the standard insulator with a ferroelectric insulator of the right thickness it should be possible to implement a step-up voltage transformer that will amplify the gate voltage thus leading to values of $S$ lower than 60 mV/decade and enabling low voltage/low power operation. The voltage transformer action can be understood intuitively as the result of an effective negative capacitance provided by the ferroelectric capacitor which arises from an internal positive feedback that in principle could be obtained from other microscopic mechanisms as well. Unlike other proposals to reduce $S$ this involves no change in the basic physics of the FET and thus does not affect its current drive or impose other restrictions.

3:42PM S2.00003 Nanowire Impact Ionization FETs, MIKAEL BJORK, IBM Research Zurich — One limiting factor in the scaling of transistor technology is the room temperature limit of 60 mV/decade of the inverse sub-threshold slope. As supply- and threshold voltages are scaled down leakage currents rise exponentially causing the standby power of highly integrated circuits to suffer. New types of devices based on band-to-band tunneling [1] or impact ionization [2] have recently been demonstrated that can circumvent the 60 mV/decade limit thereby offering lower leakage currents. We have demonstrated vertical integration [3] of a single surround-gated silicon nanowire field-effect transistor (NW FET) having an inverse sub-threshold slope as low as 6 mV/decade at room temperature that spans four orders of magnitude in current [4]. The transistor shows slopes below 60 mV/decade for supply voltages above 2 V. Due to the use of a top Schottky contact and two ungated regions the devices show ambipolar characteristics with impact ionization for both electron and hole branch. The rather small voltages reduce hot carrier injection into the gate dielectric making threshold voltage shifts and degradation of the performance minimal.


4:18PM S2.00004 Nanoelectromechanical switches, MARC BALDO, MIT, Department of Electrical Engineering and Computer Science — Power dissipation is perhaps the most important problem confronting the electronics industry. To address this issue, we investigate vertical nanoelectromechanical (NEM) switches suitable for complementary logic, reconfigurable interconnects, and static power management. NEM switches have the following advantages: (i) Near elimination of source-drain static tunneling losses, (ii) Improved subthreshold characteristics [1]— allowing lower operating voltage and hence lower dynamic power dissipation, (iii) Ability to run at much higher temperatures than Si-based CMOS. Our approach employs a carbon nanotube-based relay. We have prototyped this approach by inserting a tube into an etched gap between two contacts. Using a nanopositioner to align the tube, the prototype has demonstrated multiple switching at 5V. We will characterize this device and also integrated NEM switches.


4:54PM S2.00005 One-dimensional semiconductors for low-power electronic applications, JOERG APPENZELLER, School of Electrical and Computer Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47906 — Power dissipation is rapidly increasing from one to the next generation of silicon CMOS based chips. While following the ideal scaling rules should improve the performance without significantly increasing the power consumption, in particular the supply voltage has not been reduced in the past as required. Since the gate oxide thickness (SiO(N) in common CMOS applications) on the other hand has been decreased substantially, gate leakage currents have become a severe problem when the transistor is turned off. For logic applications, part of the applied voltage is used to switch the device from its off-state into its on-state while the other portion is used to drive the transistor into a regime of high transconductance. When asking the question about how to decrease the supply voltage to reduce power consumption of the device, both states have to be taken into account. Considering that currently more than 3 orders of magnitude current change are required to ensure proper circuit operation, already around 200mV of the supply voltage are used towards driving the transistor from the off-state to the on-state. This is true for charge-based devices that control current transport by means of a gate dependent barrier that can only be overcome by thermal emission. Those types of devices are characterized by an inverse subthreshold slope larger than around 60mV/dec. Altering the logic state by applying smaller voltages is highly desirable. My presentation will elucidate on the possibility of using band- to-band tunneling in carbon nanotubes as a viable approach to address both of the above aspects – the transistor off- and on-state performance. I will use the example of carbon nanotube based devices to discuss various switching concepts in these low-dimensional geometries and to argue why a certain device structure should be favored over another.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S3 GSNP: Aging, Shear and Rejuvenation: Mechanics of Glasses, Colloids and Granular Matter Morial Convention Center RO2 - RO3

2:30PM S3.00001 Jamming: Relating Shear and Effective Temperature1, TOM HAXTON, Department of Physics, University of Pennsylvania — In an equilibrium system, temperature not only influences the average properties of a system, such as its pressure or density, but also controls the fluctuations around those averages. In systems driven far from equilibrium, however, temperature is no longer well-defined, and fluctuations can be non-thermal in origin. I will discuss a class of such systems, namely steadily-sheared glasses, for which there is a considerable body of evidence that the idea of an effective temperature is useful, at least in certain regimes. Using nonequilibrium molecular dynamics simulations, we have now calculated seven different definitions that yield a consistent value for the effective temperature, which can be many orders of magnitude higher than the bath temperature. However, if we want to understand the behavior of a material, measuring its temperature is only a start. I will discuss recent results that show that when shear-induced fluctuations dominate over thermal fluctuations, the effective temperature controls materials properties such as the rheology and the extreme slowing down of the dynamics as the system jams.

1Supported by NSF-DMR-0605044
3:06PM S3.00002 Simulations of shear banding in metallic glasses. — Metallic glasses represent a promising high strength material, but their use is limited by the onset of a shear banding instability when their material strength is exceeded. Recent simulation studies of the initiation and development of localized deformation in molecular dynamics simulations of a number of amorphous systems reveal the structural changes that accompany plastic deformation and localization involve a decrease in the local short range ordering. We have simulated both two-dimensional and three-dimensional systems in nanoindentation [1,2], uniaxial tension [3] and compression [4] in plane strain. The degree of strain localization depends sensitively on the quench rate during sample preparation, with localization only arising in more gradually quenched samples. A systematic analysis of simulated systems in simple shear geometries [5] reveals that a Boltzmann-like relationship between strain rate and structure holds over large variations in both the applied strain rate and the initial structural state of the glass. Scaling is observed over eight orders of magnitude in strain rate. The consequences of this scaling for constitutive models of glass plasticity will be discussed.


1Supported by the National Science Foundation under award #0135009.

3:42PM S3.00003 Single particle dynamics of aging in colloidal systems. — When a liquid is quenched to form a glass it becomes trapped in a non-equilibrium state, and many of the system’s properties depend on the time elapsed since the quench. This phenomenon is known as aging. We study concentrated colloidal suspensions, a model system which has a glass transition when the particle concentration is increased. We use an optical confocal microscope to view the motion of these colloidal particles in three dimensions. Aging is most commonly detected by measuring the evolution of variables (such as the mean squared displacement) averaged over the entire system, but these quantities cannot yield information about the detailed, structural changes that occur during aging. In contrast, confocal microscopy lets us study the relationship between local structure and the motion of the colloidal particles, in both monodisperse and binary colloidal glasses. We find that particle motion occurs in cooperative groups, and that this motion is facilitated by the relatively poor packing of the particles in these regions. Work done with G. C. Cianci, J. M. Lynch, and R. E. Courtland.

4:18PM S3.00004 Aging dynamics and the mechanical behavior of glassy solids. — Aging dynamics and yielding also modify aging. This talk will present a series of molecular simulations that provide new insight into the complex, microscopic origins of the elastoplastic behavior of amorphous matter and its relationship to the macroscopic material response. In particular, we investigate the interplay between aging and plastic deformation in coarse-grained models for polymeric and metallic glasses. Molecular dynamics simulations are used to determine the macroscopic shear yield stress as well as the compliance of the model glasses for different loading conditions, temperatures, strain rates and aging times, as well as reveal their relationship to the underlying microscopic distribution of relaxation times. As in experiments on polymer glasses, we find that large stresses can decrease relaxation times and cause mechanical rejuvenation. Furthermore, we find new behavior when the aging glass undergoes more involved thermal protocols such as a temperature step. Phenomenological models will be developed that describe the data over a wide range of temperature, stress and strain rates. We also discuss how continuum models such as energy landscape pictures and the recently formulated shear transformation zone (STZ) theory of amorphous plasticity can account for the aging effects observed in the molecular simulations.

4:54PM S3.00005 Faults & Earthquakes as Granular Phenomena: Controls on Stick-Slip Dynamics. — Granular and continuous materials fail in fundamentally different ways, yet inherently discontinuous natural fault materials have often been modeled as continuum processes. Within a sheared or compressed granular material, the internal stresses take the form of a network of force chains. This network of strong connections among the particles is observed to be highly heterogeneous, and the magnitude of the stress varies widely over short distances. I will present the results of laboratory experiments which highlight the granular conrols on earthquake fault behavior. We perform experiments in a quasi-two-dimensional shear zone containing several thousand 5 mm circular and elliptical photoelastic plastic disks, allowing us to monitor the spatiotemporal evolution of both internal stress and strain. While the time, length, and strength scales are vastly different from the natural case, the frictional behavior is found to be in agreement. Therefore, the experiments allow us to isolate the effects of granular interactions and choice of boundary conditions on the fault behavior, through the observation of large populations of stick-slip and creep events.

Session S4 GIMS: Keithley Award Symposium Morial Convention Center 206

2:30PM S4.00001 Keithley Award Talk: Pushing the limits in ARPES. — A successively higher degree of parallelity in data acquisition has dramatically increased the information rate in angle resolved photoelectron spectroscopy (ARPES). This has been coupled to resolution improvements both in angle and energy. The development leading to the present state of the art is described, and recent results are presented. To extend the field further towards higher or lower energies, as well as higher resolution or larger acceptance angles, novel techniques are needed. Some recent and ongoing developments for this purpose will be described. It is also shown that the application of these techniques can be used to overcome some limitations in energy resolution even when the angular information as such is not important.

3:06PM S4.00002 High Resolution Angle-Resolved Photoemission Studies of Correlated Electron Systems. — DAN DESSAU, Department of Physics, University of Colorado, Boulder — Bjorn Wannberg’s invention of the “angle mode” for acquiring 2-dimensional ARPES images with both high energy and angular resolution has revolutionized the way modern ARPES experiments are performed. This advance has lead to both quantitative and qualitative improvements in the resolution as well as collection efficiency. In this talk I will give a few key examples of what has become possible using this new technology for the study of correlated electron systems. Particular focus is on high Tc superconductors, including a “fingerprinting” of electron-boson couplings using the isotope effect, and recent data on colossal magnetoresistive oxides which shows the critical aspect of the orbital degrees of freedom and k-dependent electron self energies.

3:42PM S4.00003 High Resolution Angle-Resolved Photoemission Studies of Correlated Electron Systems. — A successively higher degree of parallelity in data acquisition has dramatically increased the information rate in angle resolved photoelectron spectroscopy (ARPES). This has been coupled to resolution improvements both in angle and energy. The development leading to the present state of the art is described, and recent results are presented. To extend the field further towards higher or lower energies, as well as higher resolution or larger acceptance angles, novel techniques are needed. Some recent and ongoing developments for this purpose will be described. It is also shown that the application of these techniques can be used to overcome some limitations in energy resolution even when the angular information as such is not important.
4:18PM S4.00004 Angle-Resolved Photoemission Study of High Temperature Superconductors

ZHI-XUN SHEN, Stanford University — As a hybrid of spectroscopy and scattering experiments, angle-resolved photoemission spectroscopy reveals the direction, the speed, and the scattering mechanism of valence electrons. In the past two decades, enormously improved resolution and carefully matched experiments have elevated this technique to an important many-body spectroscopy. Today, ARPES experiments help setting the intellectual agenda by testing new ideas, discovering surprises, and challenging orthodoxies. This technique is at the focal point of the necessary debates leading to new paradigms of physics represented by the high temperature superconductors. In this talk, we will survey the progress of this field over the last two decades and the information we gained about the high temperature superconductors. However, the focus will be the latest ARPES data on the following subjects: i) New temperature and doping dependent data that provide insights on the relationship between pseudogap and superconducting gap; ii) New data on the Fermi surface dependent pairing and many-body interactions in self-doped multilayer cuprates. If time permits, we will also present new time resolved photoemission data from charge density wave systems.

3:06PM S5.00002 Optical sum rules for the interband MCD spectrum

The sum rule with \( p = 0 \) is the dichroic counterpart of the familiar \( f \)-sum rule for linearly-polarized light. I will show that it yields a contribution to the ground-state orbital magnetization which in insulators is associated with the circulation of the Wannier orbitals around their centers (more precisely, to the gauge-invariant part thereof). This differs from the net circulation, or total orbital magnetization, which has two additional contributions: (i) the remaining Wannier self-rotation, and (ii) the “itinerant” circulation arising from the center-of-mass motion of the Wannier orbitals. Contributions (i) and (ii) are not separately meaningful, since their individual values depend on the particular choice of Wannier functions. Their sum is however gauge-invariant, and can be inferred from a combination of gyromagnetic and magneto-optical experiments. The \( p = 1 \) sum rule is the dc limit of the dichroic Kramers-Kronig relation which yields \( \Delta \sigma \). The Karplus-Luttinger AHC. Ab-initio studies have shown that it is necessary to sample over millions of \( k \)-points to converge the calculation of this quantity. I will discuss recent first-principles calculations for ferromagnets as well as field-polarized solid and liquid heavy metals. The possible role of configurational disorder in enhancing the field-induced AHC of liquid metals by introducing low-frequency Drude-related features in the MCD spectrum will be explored.

3:42PM S5.00003 A converse approach to the calculation of NMR shielding tensors

TIMO THONHAUSER, Massachusetts Institute of Technology — We propose an alternative approach for computing the NMR response in periodic solids that is based on a recently developed theory of orbital magnetization [1]. Instead of obtaining the shielding tensor from the response to an external magnetic field, we derive it directly from the orbital magnetization appearing in response to a microscopic magnetic dipole [2]. Our new approach is very general, and it can be applied to either isolated or periodic systems. The converse procedure has an established parallel in the case of electric fields, where Born effective charges are often obtained from the polarization induced by a sublattice displacement instead of the force induced by an electric field. Our novel approach is simple and straightforward to implement since all complexities concerning the choice of the gauge origin are avoided and the need for a linear-response implementation is circumvented. We have demonstrated its correctness and viability by calculating chemical shieldings in simple molecular systems, finding excellent agreement with previous theoretical and experimental results. Applications to more complex systems are currently in progress.

1Work supported by the DOE Office of Basic Energy Sciences and National Science Foundation.
2Supported by NSF of China, NSF, DOE and Welch Foundation.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S5 DCMP: Theory of Orbital Magnetization and Related Properties Morial Convention Center R01

2:30PM S5.00001 Theory of Orbital Magnetization and its Generalization to Interacting Systems

JUNREN SHI, Institute of Physics, Chinese Academy of Sciences, China — Recently, a new formula for the orbital magnetization was proposed. In this talk, I will review the original derivation of the formula based on the semi-classical wave-packet dynamics, as well as a general derivation based on the standard perturbation theory of quantum mechanics. The quantum derivation clarifies the origin of the novel aspects of the semi-classical derivation, such as the Berry phase correction to the density of states. It is valid for general systems including insulators with or without a Chern number, metals at zero or finite temperatures. More importantly, we are able to combine the quantum derivation with the exact current and spin density functional theory (SCDFT), proving the validity of the formula for interacting systems. With this development, the new magnetization formula, in combination with the recent advances in the construction of optimized effective potential for SCDFT, will turn out to be a powerful practical tool for the study of systems that have long defied traditional ab-initio methods.


4:18PM S5.00004 Non-perturbative ab-initio calculation of the g-tensor in periodic boundary conditions, DAVIDE CERESOLI, SISSA, Trieste — Electron Paramagnetic Resonance (EPR) spectroscopy is one of the most powerful and versatile analytic tools in materials science today. The wealth of important information available from EPR spectroscopy, however, cannot be extracted from experiments alone, rather from the combination of experimental date and theoretical calculations. To date, first principle methods for computing the EPR g-tensor rely on the linearization of the effective spin Hamiltonian with respect to spin orbit (SO) coupling [1]. While this approach gives good results for light atoms, it is insufficient when SO coupling is strong, as in transition metal compounds. We have derived a method to calculate the electronic g-tensor of paramagnetic defects from first principles in a non-perturbative way, based on the formula for the orbital magnetization [2]. The main advantage of his method, is that the external magnetic field do not enter the formula explicitly, showing that the g-tensor can be calculated as a ground state quantity by including the spin-orbit term in the SCF hamiltonian. We have found a perfect agreement with linear response calculations for bulk systems and molecular complexes containing light atoms. For heavier atoms, the agreement with experimental data is substantially improved.


4:54PM S5.00005 First-principles approach to Non-Collinear Magnetism: towards Spin Dynamics, E.K.U. GROSS, Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195, Germany — Most formulations of spin density functional theory (SDFT) restrict the magnetization vector field to have global collinearity. Nevertheless, there exists a wealth of strong non-collinearity in nature, for example molecular magnets, spin-spirals, spin-glasses and all magnets at finite temperatures. The local spin density approximation (LSDA) can be extended to these non-collinear cases [1] but this extension has the undesirable property of having the exchange-correlation (xc) field parallel to the magnetization density at each point in space. When used in conjunction with the equation of motion for the spin magnetization in the absence of spin currents and external fields [2,3], this local collinearity eliminates the torsional term, resulting in no time evolution. This severe shortcomings of LSDA, where the physical prediction is qualitatively wrong, opens up an important new direction for the development of functionals where this time evolution is correctly described. Towards this goal, I will describe our extension of the Kohn-Sham optimized effective potential (OEP) method to the non-collinear case and derive the corresponding integral equations, applicable to both finite and extended systems [3,4]. Most importantly I'll show that the resulting magnetization and xc field are not locally collinear to each other for real solids, and will therefore produce manifestly different spin-dynamics.


Wednesday, March 12, 2008 2:30PM - 4:54PM – Session S6 DCMP: Superfluid Density in Underdoped Cuprates Morial Convention Center RO4

2:30PM S6.00001 Quantum critical behavior in the superfluid density of strongly underdoped ultrathin copper oxide films, THOMAS LEMBERGER, The Ohio State University — The relationship between transition temperatures $T_C$ and superfluid densities $n_S(0)$ of cuprate superconductors has been a central issue in cuprate superconductivity from the beginning. When mobile holes are removed from optimally doped CuO$_2$ planes, $T_C$ and $n_S(0)$ decrease in a surprisingly correlated fashion. Recent measurements of the superfluid density of strongly underdoped YBa$_2$Cu$_3$O$_{7-\delta}$ films and crystals have found a square-root scaling, $T_C \propto n_S(0)^{\alpha}$ where $\alpha \approx 1/2$, which supplants the approximately linear proportionality that had been deduced long ago from less underdoped samples by Uemura et al. and had been ascribed to the quasi-2D structure of cuprates. This situation leads back to a basic question – what is the behavior of the fundamental structural unit, namely, a single CuO$_2$ layer or bilayer, which is truly two-dimensional by construction? To address this question, we studied 2D samples near the critical doping level where superconductivity disappears. We measured $n_S(T)$ in films of Y$_{1-x}$Ca$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ as thin as two CuO$_2$ bilayers. $T_C$’s were as low as 3 K. We observed the 2D Kosterlitz–Thouless–Berezinski drop in $n_S$ at $T_C$, and we recovered the linear scaling $T_C \propto n_S(0)^{1/2}$ expected in 2D due to fluctuations in the phase of the superconducting order parameter. Taken together, results on 3D and 2D samples suggest that the disappearance of superconductivity with underdoping is ultimately due to quantum fluctuations near a quantum critical point.

*Work performed with I. Hetel and M. Randera; supported in part by NSF-DMR.*

3:06PM S6.00002 Superfluid density in the underdoped cuprates, DAVID BROUN, Simon Fraser University — This abstract not available.

3:42PM S6.00003 Two energy scales and the nodal-antinodal dichotomy in underdoped superconducting cuprates, ANTOINE GEORGES, CNRS and Ecole Polytechnique — Recent electronic Raman scattering experiments on hole-doped cuprates in the underdoped regime reveal that nodal and antinodal regions behave in very different manners. I will present the conclusions of a theoretical analysis of these experiments, based on a new sum-rule, and on Fermi liquid and phenomenological considerations, which lead to the conclusion that the superconducting state involves a hitherto hidden energy scale, which has the same doping-dependence than the superconducting transition temperature, in contrast to the pseudogap energy scale.

4:18PM S6.00004 Algebraic charge liquids and the underdoped cuprates, SENTHIL TODADRI, MIT — We describe a possible theoretical route for the evolution with doping of an antiferromagnetic Mott insulator into a gapless d-wave superconductor. Central to this description are “algebraic charge liquids” with power law correlations of gapless, spinless, charge e fermions. Based on this understanding a specific theory of the underdoped cuprates that naturally explains a number of puzzling phenomena including the doping and temperature dependence of the superfluid density, the photoemission spectra, and Shubnikov-de Haas oscillations is proposed. Experiments to test the theory are suggested.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S7 FGSA: Panel Discussion: Non-traditional Careers for Physicists Morial Convention Center R05
3:30PM S8.00006 Viscosity of confined suspensions. PHILIPPE PEYLA, JOHANN DAVIT, CLAUDE VERDIER, Université Joseph Fourier – Grenoble, LSP – CNRS – DYFCOM TEAM — In this work, we study experimentally and numerically the viscosity of non-brownian confined suspensions of hard spherical particles confined between two walls in a shear flow. By varying the wall-to-wall distance (gap), we show that the viscosity decreases with the gap. The deviation from this behavior is enhanced for smaller gaps. More precisely, when the wall-to-wall distance decreases, the linear term in volumic fraction decreases, which becomes increasingly shear banded with shear rate. We also confirm previous findings that monodisperse foam layers exhibit rate-independent viscosity profiles, which are quantitatively captured in a model that balances the viscous drag forces in the foam, provided that we assume the average drag force to be proportional to the number of bubbles in disordered foams.

3:42PM S8.00007 Rate dependence, drag balance and role of disorder in linearly sheared foams. GIJS KATGERT, MATTHIAS E. MÖBIUS, MARTIN VAN HECKE, Kamerlingh Onnes Laboratory, Leiden University — We linearly shear a bidisperse foam monolayer sandwiched between a glass plate and a fluid surface over 3 orders of magnitude in driving velocity. We find strongly rate-dependent velocity profiles, which become increasingly shear banded with shear rate. The shear rate is an important parameter for the shear modulus of the foam. We confirm previous findings that monodisperse foam layers exhibit rate-independent velocity profiles. We observe a transition from a 3D configuration to a quasi-2D one when the wall-to-wall distance becomes smaller than twice the spheres diameter. We find that the effective shear modulus for two particles which move perpendicularly to their connecting line is enhanced for smaller gaps. More precisely, when the wall-to-wall distance decreases, the linear term in volumic fraction decreases, which becomes increasingly shear banded with shear rate. We also confirm previous findings that monodisperse foam layers exhibit rate-independent viscosity profiles, which are quantitatively captured in a model that balances the viscous drag forces in the foam, provided that we assume the average drag force to be proportional to the number of bubbles in disordered foams.

3:54PM S8.00008 Shear Modulus of a Depletion-Induced Colloidal Gel. CHANJOONG KIM, DAVID A. WEITZ, Department of Physics and HEAS, Harvard University — Mechanical properties of a colloidal gel are of great interest because they are related to the processability of the colloidal dispersion and its stability. We measure the shear modulus for colloidal gel networks induced by depletion attraction and determine the relationship between the strength of the depletion attraction and the magnitude of the shear modulus.

4:06PM S8.00009 ABSTRACT WITHDRAWN

4:18PM S8.00010 Irreversible flow-induced vitrification of nanoemulsions by extreme droplet rupturing. JAMES N. VILKING, Dept. of Chemistry, University of California- Los Angeles, THOMAS G. MASON, Deps. of Physics and Chemistry, University of California- Los Angeles — Some materials weaken through fracturing when subjected to extreme stresses. However, breaking down repulsive bits of condensed matter that are dispersed in a viscous liquid can also potentially cause a dramatic and irreversible increase in the dispersion’s elasticity. Here, we demonstrate this principle using dispersions of one liquid in another immiscible liquid. Anionically stabilized microscale emulsions are subjected to a history of stresses, and we demonstrate that the dispersed phase can undergo a dynamical phase transition from an absorbing reversible steady state to a fluctuating irreversible state. For a given strain amplitude $\gamma$, this transition occurs at a critical volume fraction $\phi_c$. However, if the particles are not neutrally buoyant, they either sink to the bottom or float to the top of the container. New experiments and simulations show that under periodic shear, the particles resuspend, and that for a given strain amplitude $\gamma$, the particles evolve towards the critical concentration $\phi_c$ without any external intervention. In that case, particle collisions nucleated at the bottom of the shear cell propagate through the sample and keep the system suspended close to the critical volume fraction $\phi_c$.$\gamma$. Hence, slowly sedimenting particles under oscillatory shear appear as a new class of self-organized critical systems hitherto unreported.

4:42PM S8.00012 Self-organized criticality of slowly sedimenting shear suspensions. WEINING MAN, LAURENT CORTE, Physics Department, New York University, SHARON GERBODE, Department of Physics, Cornell University, DAVID PINE, PAUL CHAIKIN, Physics Department, New York University — Suspensions of neutrally buoyant particles driven by slow periodic shear can undergo a dynamical phase transition from an absorbing reversible steady state to a fluctuating irreversible state. For a given strain amplitude $\gamma$, this transition occurs at a critical volume fraction $\phi_c$. However, if the particles are not neutrally buoyant, they either sink to the bottom or float to the top of the container. New experiments and simulations show that under periodic shear, the particles resuspend, and that for a given strain amplitude $\gamma$, the particles evolve towards the critical concentration $\phi_c$ without any external intervention. In that case, particle collisions nucleated at the bottom of the shear cell propagate through the sample and keep the system suspended close to the critical volume fraction $\phi_c$. Hence, slowly sedimenting particles under oscillatory shear appear as a new class of self-organized critical systems hitherto unreported.

4:54PM S8.00013 Random organization: A dynamical phase transition. LAURENT CORTE, DAVID J. PINE, PAUL M. CHAIKIN, Center for Soft Matter Research, NYU — We introduce a simple model motivated by recent experiments in sheared suspensions. We show that randomly dispersed colloidal particles are sufficient to generate an organized state where further collisions are suppressed. This organization by self-activated random walkers presents a much more efficient process than when all particles are diffusing. It only occurs provided that the density in particle is lower than a critical value $p_c$ and is characterized by a dynamical phase transition. A mean-field description captures the existence of this transition. It suggests that the value of $p_c$ is determined by the ratio $p_c / p_s$, where $p_s$ is the probability that a “quiet” particle be collided. Our results also reveal that the ordering can be enhanced by straining the system periodically. However, these more organized states become less and less accessible as the strain amplitude is increased.
5:06PM S8.00014 X-ray photon correlation spectroscopy in a shear flow, ANDREI FLUERASU, European Synchrotron Radiation Facility — X-ray photon correlation spectroscopy was used to measure the diffusive dynamics of colloidal suspensions in a shear flow. The results presented here show how the intensity autocorrelation functions measure a coupling between the diffusive dynamics of the particles and their flow-induced, convective motion. However, in the limit of low flow/shear rates, it is possible to obtain the diffusive component of the dynamics. The conditions under which this is possible are easier to achieve at higher values of the scattering wavevector q and this may provide an advantage of X-ray over, for e.g. light, photon correlation spectroscopy. In recent work (A. Fluerasu et al., submitted, 2007) we have shown this result to hold for dillute (particle volume fraction Φ up to 50 %) suspensions when the correlation functions probe, basically, the self-diffusion of individual, non-interacting particles. Here we will also adress the collective motion of concentrated suspensions of hard-sphere systems (Φ up to 50 %) and study the coupling between the shear-induced response and the collective diffusion of the suspension. An important benefit of this experimental strategy over more traditional X-ray methods, is the minimization of X-ray induced beam damage, which makes the method suitable for the study of the dynamical properties of a large class of complex soft-matter and biological fluids.

5:18PM S8.00015 Electrophoretic “Equilibrium” Profile of Charged Colloids, ROMAIN PLANQUES, PAUL CHAIKIN, Dept. of Physics, New York University — We perform an electrophoresis experiment of a concentrated colloid against a semipermeable membrane. The electric field forces the charged particles against the membrane and sets up a concentration profile similar to that of a colloid in gravitational sedimentation equilibrium where gravitational forces compete against the osmotic pressure gradient. In the present case there is a current which flows through the electrolyte so the system reaches a steady state profile rather than equilibrium. The electric field, colloid and ionic concentrations adjust self consistently to produce the profile. We use 91 nm polystyrene spheres with sufficient charge that they crystallize and observe their Bragg scattering as a function of height to determine the lattice spacing and particle concentration. We also use 700nm spheres and obtain their concentration profile with X-ray absorption. The fluid flow is zero for a capped system. Connecting a return tube from the supernatant side above the electrophoretic sediment to below the filter yields an electroosmotic flow and circulation. The profile changes substantially and allows us to study the hydrodynamic interactions as a function of concentration for the electrophoresing particles.

Wednesday, March 12, 2008 2:30PM - 5:30PM — Session S9 DCMP: Optical Properties of Superconductors Morial Convention Center R07

2:42PM S9.00002 Investigation of the bosonic spectral density in highly under-doped YBa$_2$Cu$_3$O$_{6.35}$, JING YANG, THOMAS TIMUSK, Department of Physics and Astronomy, McMaster University, DOUGLAS BONN, RUIXING LIANG, WALTER HARDY, Department of Physics and Astronomy, University of British Columbia — We studied the doping dependence of the bosonic spectral function in nearly optimally-doped LSCO and highly under-doped YBa$_2$Cu$_3$O$_{6.35}$ single crystals by optical spectroscopy. With fixed oxygen content, the hole doping of the YBCO system can be fine-tuned by varying the degree of oxygen ordering. After annealing and quenching, we were able to make oxygen less ordered and obtain a highly under-doped YBa$_2$Cu$_3$O$_{6.35}$ sample with a very low transition temperature around 18K (about 20% of the optimal T$_c$). The a-axis reflectance data of this sample at nine temperatures between 30K and 295K was measured with an infrared spectrometer between 60 and 40 000 cm$^{-1}$ with the aid of three different infrared and optical polarizers. The optical properties of the highly under-doped YBCO sample show dramatic changes compared to the ortho-II YBCO sample. The strong sharp mode in the bosonic spectral function $\alpha^2 F(\Omega)$ in the ortho-II YBCO is absent in the highly under-doped sample.

2:54PM S9.00003 Optical conductivity of electron-doped cuprates, pseudogap and antiferromagnetic fluctuations, D. BERGERON, B. KYUNG, V. HANKEYCH, A.-M.S. TREMBLAY, Universite de Sherbrooke — Recent neutron scattering experiments on electron-doped cuprates have shown that the antiferromagnetic correlation length at the pseudogap temperature scales like the thermal de Broglie wavelength. This result, predicted by the Two-Particle Self-Consistent approach (TPSC), suggests that antiferromagnetic fluctuations are at the origin of the pseudogap in electron-doped cuprates. Clearly one needs to verify that other physical properties can also be explained within the same formalism. We thus derived, within TPSC, the formula appropriate for optical conductivity, including the first vertex correction. Our numerical calculations then show that, as observed experimentally, there is a transfer of spectral weight from low to high energy when antiferromagnetic fluctuations become important near the pseudogap temperature.

3:06PM S9.00004 Optical Properties of Organic Superconductor $\kappa$-(BETS)$_2$FeBr$_4$, M. REEDYK, N. HOSSEIN KHAIH, B. LIU, G.V. SUDHAKAR RAO, Brock University, St. Catharines, Canada, H. FUJIIWARA, Osaka City University, Japan, H. KOBAYASHI, M.A. TANATAR, K. YAKUSHI, T. NAKAMURA, Institute for Molecular Science, Okazaki, Japan — The optical response to far- and mid-infrared radiation has been measured for quasi two-dimensional plate-shaped crystals of $\kappa$-(BETS)$_2$FeBr$_4$ [where BETS = bis(ethylenedithio)-tetraselenafulvalene]. $\kappa$-(BETS)$_2$FeBr$_4$ is the first antiferromagnetic organic superconductor at ambient pressure with Néel temperature $T_N \approx 2.5$ K and superconducting transition temperature $T_c \approx 1.1$ K. Polarized thermal reflectance measurements were performed to compare the reflectance above and below $T_c$ and $T_N$ using a Martin-Puplett-type polarizing interferometer and $^3$He cryostat. In addition polarized absolute reflectance measurements in the far- and mid-infrared were carried out at temperatures in the natural state between 4 K and 300 K using a Michelson interferometer and cold finger cryostat. Kramers-Kronig analysis was then used to determine the optical conductivity of $\kappa$-(BETS)$_2$FeBr$_4$ at these temperatures.

1This work was supported by the DOE under contract number DE-AC02-98CH10886.

2Supported by NSERC, CFI, MEQ, CIFAR and the CRC program

3This work is supported by NSERC Canada.

4currently at the University of Sherbrooke
3:18PM S9.00005 Optical properties of lattice/spin polarons in underdoped cuprates, SIMONE FRATINI, Institut Neel - CNRS, Grenoble, France, SERGIO CIUCHI, Research Center SMC, INFM-CNRS and Dept. Physics, Universita' dell'Aquila, I-Aquila, Italy, EMMANUELLE CAPPELLUTI, Research Center SMC, INFM-CNRS and Dept. Physics, Universita La Sapienza, Rome, Italy — In this contribution we investigate the optical spectra of one hole in the Holstein-\(J\) model. We employ a dynamical mean-field theory which becomes exact in the limit of infinite connectivity. This allows us to investigate the local (incoherent) features which are related to the internal structure of the polaron, disregarding coherent motion which might be reflected in the Drude-like peak. We show that magnetic and electron-phonon interactions sustain each other in establishing polaronic regime. Polaron formation is reflected in a peculiar mid-infrared (MIR) band which is however notably different in the case of a lattice or magnetic origin. The dependence of \(n(\omega)\) on the electron-phonon coupling constant \(\lambda\), on the exchange interaction \(J\) and on temperature \(T\) is investigated. We compare our results with experimental data in \(\text{Nd}_2\text{CuO}_4\) showing that the doping and temperature dependences of the optical conductivity in this compound is naturally reproduced by a spin/lattice polaronic model.

3:30PM S9.00006 Optical Conductivity and Correlation Strength of the High \(T_c\) Cuprate Superconductors, MASSIMO CAPONE, SMC, CNR-INFM and Dip. di Fisica, University of Rome “La Sapienza”, Piazzale A. Moro 2, I-00185, Rome, Italy, ARMIN COMANAC, Department of Physics, Columbia University, 538 W. 120th Street, New York, NY, LUCA DE’ MEDICI, Department of Physics, Rutgers The State University of NJ, 136 Frelinghuysen Road, Piscataway, NJ 08854, ANDREW MILLIS, Department of Physics, Columbia University, 538 W. 120th Street, New York, NY — High temperature copper-oxide-based superconductivity is obtained by adding carriers to insulating “parent compounds.” It is widely believed the parent compounds are “Mott” insulators, in which the lack of conduction arises from anomalously strong electron-electron repulsion, and that the unusual properties of Mott insulators are responsible for high temperature superconductivity. This paper presents a comparison of optical conductivity measurements and theoretical calculations based on Dynamical Mean-Field Theory which challenges this belief: the analysis indicates that the correlation strength in the cuprates is not as strong as previously believed, that the materials are not properly regarded as pure Mott insulators, that antiferromagnetism is essential to obtain the insulating state and, by implication, that antiferromagnetism is essential to the properties of the doped metallic and superconducting state as well.

3:42PM S9.00007 Is the Optical Sum Rule Violated in Cuprates?1, MICHAEL NORMAN, Materials Science Division, Argonne National Lab, ANDREY CHUBUKOV, Dept. of Physics, University of Wisconsin, Madison, ERIK VAN HEUMEN, ALEXEY KUZMENKO, DIRK VAN DER MAREL, University of Geneva, Switzerland — Much attention has been given to a possible violation of the optical sum rule in the cuprates, and the connection this might have to kinetic energy lowering. The true optical integral is composed of a cut-off independent term (whose temperature dependence is a measure of the sum rule violation), plus a cut-off dependent term that accounts for the extension of the Drude peak beyond the upper bound of the integral. We find that optical data in the normal state of the cuprates can be accounted for solely by the latter term, implying that the dominant contribution to the observed sum rule violation in the normal state is due to the finite cut-off.

1Work supported by the DOE, Contract No. DE-AC02-06CH11357, NSF-DMR 0604406, the Swiss NSF and NCCR-MaNEP.

3:54PM S9.00008 Sum rule analysis of \(\text{YBa}_2\text{Cu}_3\text{O}_y\) in magnetic field, ANDREW LAFORE, Univ. of California, San Diego, WILLIE PADILLA, Boston College, KENNETH BURCH, Los Alamos National Laboratory, ZHIQIANG LI, ALEXANDER SCHAFGANS, Univ. of California, San Diego, KOUI SEZAWA, YOICHI ANDO, Osaka University, Japan, DIMITRI BASOV, Univ. of California, San Diego — We present infrared magneto-optical reflectance measurements which characterize the interplane transport of three dopings of \(\text{YBa}_2\text{Cu}_3\text{O}_y\). An optical sum rule analysis reveals the field-evolution of the energy scale from which the superconducting condensate is drawn. We find that fields applied parallel to the \(c\) axis totally suppress high-energy contributions to the condensate in underdoped samples while only moderately reducing the superfluid density. For optimally doped crystals the sum rule is satisfied and not modified by field. These results point toward a more conventional, BCS-like condensation mechanism, and will be discussed in relation to the interlayer phase coherence.

4:06PM S9.00009 Illustration of advantages of optical self-energy for understanding conductivity data on superconductors, E.J. NICOL, University of Guelph, J.P. CARBOTTE, McMaster University — Over the last 20 years, it has become common to present optical data on exotic superconductors, such as high \(T_c\), and heavy fermions, in terms of a generalized optical self-energy. However, this quantity has never been fully examined in the context of conventional superconductivity and tested against experiment. We present a detailed study of the optical scattering rate and mass renormalization with emphasis upon the role of elastic and inelastic scattering, and make comparison with recent high quality data. This illustrates the usefulness of this approach and the new insights that can be obtained.

4:18PM S9.00010 Optical properties of underdoped high \(T_c\) superconductors from a phenomenological model, E. ILLES, E.J. NICOL, University of Guelph, J.P. CARBOTTE, McMaster University — We calculate the optical conductivity predicted by a phenomenological model for the pseudogap state given by Yang, Rice and Zhang [1]. In particular, we present results for both pseudogap and superconducting states as a function of doping. In addition to the conductivity, we examine the optical self-energy (i.e. the optical scattering rate and mass renormalization) and discuss our results in light of experiment.


4:30PM S9.00011 Signatures of superconducting gap inhomogeneities in the optical conductivity, J. LEBLANC, E.J. NICOL, University of Guelph, J.P. CARBOTTE, McMaster University — The observation of energy gap inhomogeneities in the \(\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_2\text{O}_{8+\delta}\) high \(T_c\) cuprates motivates studying such effects on other properties. We have calculated the optical conductivity using an effective medium approximation to mix superconducting regions with different energy gaps. We present our results and comment on possible signatures in the conductivity and optical self-energy.

4:42PM S9.00012 Time resolved Raman scattering on the pair-breaking peak in Bi-2212 — direct observation of the dynamics of the superconducting order parameter, PELANGI SAICHU, ILKA MAHNS, ARNE GOOS, STEPHAN BINDER, STEFAN SINGER, University of Hamburg, J. UNTERHINNINGHOFS, Max-Planck Institut fuer Festkoerperforschung, BENJAMIN SCHULZ, ANDRIVO RUSYDI, University of Hamburg, S.L. COOPER, M.V. KLEIN, University of Illinois at Urbana-Champaign, P. GUPTASARMA, University of Wisconsin-Milwaukee, DIRK MANSKE, Max-Planck Institut fuer Festkoerperforschung, MICHAEL RUEBHAUSEN, University of Hamburg — We employ a novel time resolved two-color pump probe Raman technique to study the electronic dynamics in the superconducting state of the high temperature superconductor Bi-2212. By studying the temporal evolution of the gap and the pair-breaking peak in the superconducting state, we reveal two contributions to the superconducting order parameter that respond within 1 ps and 7 ps, respectively. Both effects conserve spectral weight in the sense that the suppression of the pair-breaking peak appears concomitantly with the build up of in-gap states. The recovery times for both contributions to the gap are different by a factor of 4 outlining fundamentally different coupling mechanisms.
4:54PM S9.00013 Electronic Raman scattering in cuprates, WILLIAM GUYARD, Laboratoire Matériaux et Phénomènes Quantiques (Université Paris Diderot-Paris 7, CNRS), MATHIEU LE TACON, European Synchrotron Radiation Facility, MAXIMILIEN CAZA-VOYS, ALAIN SACUTO, Laboratoire Matériaux et Phénomènes Quantiques (Université Paris Diderot-Paris 7, CNRS), ANTOINE GEORGES, Centre de Physique Théorique, Ecole Polytechnique, DOROTHÉE COLSON, ANNE FORGET, Service de Physique de l’Etat Condensé, CEA-Saclay — We report electronic Raman response in mercury compound. In cuprates, the superconducting gap reaches its maximum values along the antinodal directions and vanishes along nodal directions corresponding respectively to the principal axes and the diagonal in the Brillouin zone. We will present both the antinodal $(B_{1g})$ and nodal $(B_{2g})$ responses as a function of doping and temperature. We will also report the full symmetric Raman response $(A_{1g})$ as a function of doping.

5:06PM S9.00014 Self Energy Corrections to Resonant Inelastic X-ray Scattering in the Cuprates, WAEL AL-SAWAIL, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — Resonant inelastic x-ray scattering (RIXS) is emerging as a powerful probe of strongly correlated systems by providing direct momentum-resolved information on charge excitations across the Mott gap. We have shown recently that long-range Coulomb interactions and self-energy corrections play an important role in modifying the electronic spectra of the cuprates. [1,2] Here we discuss model calculations to explore how plasmon and magnon corrections to the self-energy influence the RIXS spectra of the cuprates. [1] R.S. Markiewicz and A. Bansil, Phys. Rev. B 75, 020508(R) (2007).

1Work supported in part by the USDOE.

5:18PM S9.00015 Optical conductivity in strongly correlated electron materials, JIANMIN TAO, JIAN-XIN ZHU, Los Alamos National Laboratory — Ultrafast optical phenomena are of fundamental importance in the investigation of electronic structures of strongly correlated electron materials [1]. Starting from the Hamiltonian of a correlated electron material exposed to a time-dependent laser field, we formulate the particle current density. Within a mean-field approximation, we express the current density in terms of the expectation values of quasiparticle density operators by performing the canonical transformation. Within the Heisenberg picture, we solve a set of equations of motion for these quasiparticle densities. Finally we calculate the optical conductivity in several typical systems. [1] R. D. Averitt and A. J. Taylor, J. Phys: Condensed Matter 14, R1357 (2002).

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S10 DCMP: Superconductors: Synthesis and Physical Properties  Morial Convention Center RO8

2:30PM S10.00001 Growth of MgB$_2$ Films by an Impinging Jet HPCVD Reactor Design, DANIEL LAMBORN, Department of Chemical Engineering, Penn State University Park, PA, USA, R.H.T. WILKE, QI LI, Department of Physics, Penn State University, University Park, PA, USA, XIAOXING XI, D.W. SNYDER, SHUFANG WANG, JOAN REDWING, Department of Materials Science and Engineering, Penn State University, University Park, PA, USA — An impinging jet hybrid physical-chemical vapor deposition (HPCVD) reactor design was used for the growth of both thin and thick MgB$_2$ films. This technique was able to independently control the substrate and Mg supply temperatures, and still maintained sufficient Mg overpressure to ensure phase stability. Thin films were predominantly axis oriented with the (0001) sapphire substrate while the thick films were either polycrystalline or showed preferred orientation. This technique was able to independently control the substrate and Mg supply temperatures, and still maintained sufficient Mg overpressure to ensure phase stability. Thin films were predominantly axis oriented with the (0001) sapphire substrate while the thick films were either polycrystalline or showed preferred orientation. Thick films (~10 µm) were deposited at a growth rate of ~110 µm/hr and showed a maximum T$_c$ of 39.8 K and residual resistivity ratio of 6.6. The thick films also showed a high J$_c$ of 2x10$^6$ A/cm$^2$ at low applied magnetic fields even at 20 K. The results indicate that the impinging jet HPCVD configuration shows promise for coated conductor processes.

1 Also with Department of Physics, Penn State University, University Park, PA, USA
2 Also with Department of Chemical Engineering, Penn State University, University Park, PA, USA

2 Films Fabricated by Ex Situ Annealing of CVD-Grown B Films in Mg Vapor

2:54PM S10.00003 High isostatic pressure synthesis of sonochemically modified MgB$_2$ superconductor, BRETT MCCARTY, JOSUA HUGEN, DANIEL STOECKLEIN, RUSLAN PROZOROV, Iowa State University — A study of the effects of high intensity ultrasound on MgB$_2$ precursors with different additives to improve pinning properties is reported. Additives were either co-sonicated with boron or mixed into sonoiced boron afterwards. Hot isostatic pressure (HIP) was used to form fully dense MgB$_2$ samples from precursors. Analysis of magnetization, microstructure and x-ray diffraction will be presented.

1Supported by the DOE-BES contract No. DE-AC02-07CH11358, NSF grant No. DMR 0603841 and Alfred P. Sloan Foundation
3:06PM S10.00004 Preparation and transport measurements of high Tc disordered MgB2 thin films1. LI ZHANG, WOLTER SIEMENS, NICHOLAS BREZNAY, AHARON KULPITULNIK, MALCOLM BEASLEY. Stanford University — In this talk we present a method using pulsed laser deposition to fabricate single-layer disordered MgB2 thin films. Both Mg and stoichiometric MgB2 targets are used during the deposition. The films have been characterized by AFM, XPS, and XRD to establish the quality of the surface and the structural and compositional uniformity of the films. Though the uniformity of the films is still under investigation, transport measurements show that the films exhibit behavior characteristic of the superconductor-insulator transition at relatively high temperatures (2 to 5K). We will also review some preliminary low temperature and high magnetic field transport measurement results. Also of interest is the very low spin-orbit scattering expected in MgB2 due to the low Z of Mg and B. This work is funded by DoE and NSF.

3:18PM S10.00005 Crystal growth of superconducting materials La2-xBaxCuO4, GENDA GU, J.S. WEN, Z.J. XU, J.M. TRANQUADA, BNL — Since the discovery of the superconductivity in high temperature superconducting oxide La2-xBaxCuO4 in 1986, a large number of groups have attempted to grow the single crystals. However, no single crystal La2-xBaxCuO4 with x<0.11 has been successfully grown. In this project, the effects of the growth condition and the compositions of a feed rod on the crystal growth of La2-xBaxCuO4 has been studied by an infrared image floating zone method. The experimental result shows that a planar solid-liquid growing interface tends to break down into a cellular interface when the growth velocity is more than 1 mm/h. When the planar solid-liquid growing interface break down into a cellular interface, the single crystal size decreases abruptly and the as-grown rod is not single phase. The large single crystals of La2-xBaxCuO4 with x=0 to 0.165 has been successfully grown. The single crystals of La2-xBaxCuO4 with x=0 to 0.165 up to 6 mm diameter and 150 mm length have been grown. The superconducting transition temperature Tc of as-grown single crystals of La2-xBaxCuO4 (x=0 to 0.165) have been measured.

3:30PM S10.00006 Superconductivity in La(Ni1-xTc)2C2 (T = Cu, Ti, and Pt)1. H.H. SUNG, S.Y. CHOU, Y.C. KUNG, H.K. KUO, K.J. SYU, W.H. LEE, Department of Physics, National Chung Cheng University, Ming-Hsiung, Chia-Yi, Taiwan, ROC, W.H. LEE TEAM — LaNiC2, which crystallizes in an orthorhombic CeNiC2 type structure with space group Ann2, is the first nickel-based ternary carbide superconductor with Tc ~ 2.7 K. Published results showed that about 50% substitution of La in LaNiC2 with the 5f thorium (Th) element could enhance the superconducting critical temperature Tc up to 7.9 K. Present results of static magnetization and electric resistivity data for fifteen polycrystalline La(Ni1-xTc)2C2 (T = Cu, Ti and Pt) compounds measured in the temperature range 1.8 ~ 4.4 K and 2.0 ~ 300 K, respectively. Discussion of the improvement, with respect to pure LaNiC2, on the superconducting critical temperature Tc, will be directed toward the changes of valence, lattice parameters as well as the effects of solubility limit in the pseudoternary La(Ni1-xTc)2C2 alloys. W.H. Lee, H.K. Zeng, Y.D. Yao and Y.Y. Chen, Physica C 266, 138 (1996). V.K. Pecharsky, K.A. Gschneidner, Jr., and L.L. Miller, Phys. Rev. B 58, 497 (1998). W.H. Lee and H.K. Zeng, Solid State Commun. 102, 433 (1997).

3:42PM S10.00007 ABSTRACT WITHDRAWN

3:54PM S10.00008 Magnetron sputter deposition of a 48-member cuprate superconductor library: Bi2Sr2YxCa1−xCuO8+d (0.5 ≤ x ≤ 1) linearly varying in steps of Δx = 0.01,2. KEVIN HEWITT, ROBERT SANDERSON, Dalhousie University — Using magnetron sputtering, a spatial composition spread approach was applied successfully to obtain 48-member libraries of the Bi2Sr2YxCaxCuO8+d (0.5 ≤ x ≤ 1) cuprate superconducting system. The libraries were deposited onto (100) single crystal MgO mounted on a water cooled rotating table, using two targets: the antiferromagnetic insulator Bi2Sr2YCuO8+d (P=98 W RF) and the hole doped superconductor Bi2Sr2CaCuO8+d (P=44 W DC). A low chamber pressure of 0.81 mTorr argon is used to reduce scattering by the process gas. To minimize oxygen resputtering a substrate bias of -20 V was used as well as a process gas free of oxygen. A rapid thermal processor is used to post-anneal the amorphous deposited films in a step annealing regime - ramp at 5 ◦C/s for heating and cooling, with a first plateau at 875 ◦C held for 200 s, and a second at 875 ◦C held for 480 s. X-ray diffraction reveals that the films develop crystalline order with the c-axis lattice parameter contracting linearly from 30.55 ˚A (x=0.5) to 30.24 ˚A (x=1.0) following a step annealing regime - ramp at 5 ◦C/s for heating and cooling, with a first plateau at 875 ◦C held for 200 s, and a second at 875 ◦C held for 480 s. In addition, surface morphology and grain connectivity of the samples were degraded and the high-Tc phase of the samples decreased with increasing Gd addition. The possible reasons for the observed degradation in microstructure, superconducting and mechanical properties due to Gd addition were discussed. Supported by the National Science Council of ROC under grant no. NSC 96-0212-M-194-008-MY3.

4:06PM S10.00009 Mechanical and superconducting properties of Bi1.8Pb0.35Sr1.9Ca2.1Cu3Gd4Oy system3. MUSTAFA AKDogan, Abant Izzet Baysal University, OZGUR OZTURK, Kastamonu University, HUSEYIN AYDIN, MURAT ERMED, CABIR TERTIOGLU, Abant Izzet Baysal University — The influence of addition of the rare earth ion Gd in Bi1.8Pb0.35Sr1.9Ca2.1Cu3Gd4Oy superconductor has been investigated by varying Gd addition (x=0, 0.1, 0.2, 0.3, 0.4 and 0.5). The samples were prepared by standard solid-state reaction methods. Phase analyses of the samples by X-ray diffraction (XRD), microstructure examination by scanning electron microscopy (SEM), superconducting properties by dc electrical resistivity and mechanical properties by static indentation were carried out to assess the effects of Gd addition. These measurements indicated that the superconducting transition temperature, Vickers hardness, Young’s modulus, yield strength, fracture toughness values of the samples strongly depend on the Gd addition. The values of Ti, He, E, Y and K1IC of the samples decreased with the increase in Gd addition. The hardness values of the samples are also found to be load independent, higher than the load independent) hardness, Young’s modulus, yield strength, fracture toughness of the samples. From XRD and SEM analyses, the addition of the sample by Gd degrades formation of the high-Tc Bi-2223 phase, and surface morphology and grain connectivity in comparison with undoped sample, respectively.

4:18PM S10.00010 Investigation of Some Physical Properties of Gd added Bi-2223 Superconductors, MURAT ERMED, Abant Izzet Baysal University, OZGUR OZTURK, Kastamonu University, HUSEYIN AYDIN, MUSTAFA AKDogan, CABIR TERTIOGLU, AHMET VARILCI, IBRAHIM BELENLI, Abant Izzet Baysal University — Static microindentation, XRD, SEM, DC electrical resistivity and critical current density measurements were performed to investigate some physical properties of Bi1.8Pb0.35Sr1.9Ca2.1Cu3Gd4Oy superconducting samples with x=0.0, 0.1, 0.3, and 0.5. The indentation load versus diagonal length of the samples under different indentation loads in the range of 0.245-2.940 N were presented. The microindentation measurements showed that, for the Gd added sample, the load dependent (apparent) microhardness value (Hap) is lower in comparison with that of the pure sample(x=0). The values of Hap were found to be load dependent. In addition, we extracted the load independent (true) microhardness using the Kick’s law, proportional specimen resistance (PSR), modified proportional specimen resistance (MPSR) model and the Hays-Kendall (HK) approach and compared the true hardness with the apparent hardness. We observed from the transport measurements that addition of Gd decreased Tc and Jc. In addition, surface morphology and grain connectivity of the samples were degraded and the high-Tc phase of the samples decreased with increasing Gd addition. The possible reasons for the observed degradation in microstructure, superconducting and mechanical properties due to Gd addition were discussed.
4:30PM S10.00011 Transport macroscopic and mechanical properties of Au diffusion-doped Bi-2223 superconductors. O. OZTURK, Kastamonu Univ. C. TERZIOGLU, A. VARLICI, I. BELENLI, Abant Izzet Baysal Univ. We have investigated the effect of the gold-diffusion on the mechanical properties of the Bi-2223 superconducting samples with different annealing times (10, 20 and 50 hours). The samples are prepared by the conventional solid-state reaction method in the polycrystalline bulk form. Doping of Bi-2223 was carried out by means of gold diffusion during sintering from an evaporated gold film on pellets. The experimental works in this study consist of dc electrical resistivity measurements for electrical and superconducting properties, microhardness measurements for mechanical properties, X-ray diffraction for phase analyses and lattice parameters, and scanning electron microscopy for microstructure examination. These measurements showed that Au-doping, in comparison with the undoped samples, increased the critical transition temperature and enhanced formation of high-Tc phase. Additionally, microhardness and grain size were also improved with increasing amount of diffusion. Moreover, the diffusion-annealing time decreased the number and size of voids and increased the transition temperature. The experimental results of hardness measurements were analyzed using the Kick’s law, modified proportioned specimen resistance (MPSR) model and the Hays-Kendall (HK) approach. Among them HK approach was the most successful.

This work is supported partly by the Scientific and Technological Council of Turkey (Project No: 104T325) and partly the Turkish State Planning Organization (DPT) (Project No: 2004K120200).

4:42PM S10.00012 Critical current density variations with increasing thickness in YBa₂Cu₃O₇₋ₓ + BaSnO₃ (BSO) films. CHAKRAPANI VARANASI, University of Dayton Research Institute (UDRI), JACK BURKE, LYLE BRUNKE, UDRI, HAIYAN WANG, Texas A&M, PAUL BARNES, Air Force Research Labs, UDRI TEAM, TEXAS A&M COLLABORATION, AFRL TEAM — To increase the engineering critical current density (Jc) of YBa₂Cu₃O₇₋ₓ (YBCO) films, it is of great importance to grow thicker films with high critical current density (Jc). However, it has been shown in YBCO films that the thickness is an essential factor for the increase of Jc, which is in contradiction to the previous work by this group showed that YBCO+BaSnO₃ (BSO) films of ~ 300 nm thickness can be grown with more than an order of magnitude increase in the Jc in applied magnetic fields using a dual phase sector PLD target approach. In the present work a systematic study of Jc, dependence on the thickness of YBCO+BSO thick films was undertaken by growing different films with thicknesses ranging from 300 nm to 4 µm. The Jc of these films was measured using a magnetometer indicated that high Jc at high fields can be maintained even in thicker films. The cross-sectional TEM analyses of the thick films showed that the BSO nanocolumns grow through out the entire thickness of the samples. Microstructural details and the superconducting properties of thick YBCO+BSO films will be presented.

5:06PM S10.00014 NbN films grown by chemical solution deposition. GUEIF ZOU, MENKA JAIN, HONGMEI LUO, S. A. BAILY, T. M. MCCLEESKY, E. BAUER, A. K. BURRELL, Q. JIA, Los Alamos National Lab. MPA TEAM — NbN films were grown on quartz substrate using a chemical solution technique of polymer-assisted deposition for the first time. The precursor films were annealed at different temperatures in ammonia atmosphere. X-ray diffraction and electron microscopy analysis indicated that the films were polycrystalline. Preliminary optical spectroscopy results of these films showed several strong peaks in the visible range that can be attributed to the NbN phase. Wide peaks in the photoluminescence spectrum suggest many defects in these films. The transition temperature (measured from SQUIDs) of these films also will be discussed in this paper.

5:18PM S10.00015 Superconductivity in YbGa₃Si₂₋ₓ with the AlB₂-type structure. N. TSUJI, M. IMAI, NIMS, Japan, H. YAMAOKA, RIKEN, H. OHASHI, NIMS, Japan, D. NAMOTO, SPring-8 Service Co., I. JARRIGE, Japan Atomic Energy Agency, H. YOSHIDA, Kyoto University, H. YOSHISAKURA, H. KITAZAWA, NIMS. Japan. In the magnetic susceptibility and the specific heat of the YbGa₃Si₂₋ₓ the gap structure has been obtained. Very recently, we discovered superconductivity in the AlB₂-type compound YbGa₃(Si₂O₈) below Tc = 2.5K. We report here on the structural and electronic properties of the YbGa₃Si₂₋ₓ series. XRD and TEM/EDS analysis suggested that the AlB₂-type phase is sustained for 1.0 ≤ x ≤ 1.4. Tc is found to decrease from 2.5K for x = 1.0 to 1.9K for x = 1.3 and eventually vanish for x = 1.4. High-resolution X-ray absorption spectra across the Yb-L₁₁₁ edge measured at SPring-8 on the beamline BL15XU. The valence of Yb was estimated to be 2.3+, suggesting a predominant Yb⁴⁺ character with minor importance of 4f electrons in the superconductivity.

Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, NM 87545 (USA).

Wednesday, March 12, 2008 2:30PM - 5:30PM — Session S11 DCP: Theory of Superconductivity in Cuprates I Morial Convention Center R09

2:30PM S11.00001 Cuprate higher harmonic gap structure: theory vs. experiment. DAVID PARKER, Max Planck Institute for the Physics of Complex Systems, ALEXANDER BALATSKY, Theoretical Division, Los Alamos National Laboratory. We present a detailed comparison to experiment of the generalized gap symmetry predictions of spin-fluctuation mediated superconductivity theory in the hole-doped and electron-doped cuprates, within a weak-coupling BCS framework. We comment on the implications of these results for the ongoing “one gap vs two gap” controversy in the cuprates, and discuss the impact of these results on the quasiparticle lifetime model of the cuprate Fermi arcs.

2:42PM S11.00002 Sublattice model of atomic scale pairing inhomogeneity in a superconductor. VIVEK MISHRA, P.J. HIRSCHFELD, Department of Physics, University of Florida, Gainesville, FL 32611, YURI S. BARASH, Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow reg., 142432, Russia. We study a toy model for a superconductor on a bipartite lattice, where intrinsic microscopic inhomogeneity is produced by two different pairing couplings on a novel such sublattice. We discuss the effects of the inhomogeneity on the transition temperature, the density of states, the specific heat and superfluid density in the framework of the Bogoliubov-de Gennes equations, which may be solved analytically in several interesting cases. The phase diagram in the plane of two pairing constant is found to include a state of gapless superconductivity.
2:54PM S11.00003 Suppression of d-wave superconductivity in the weakly inhomogeneous checkerboard Hubbard Model. D.G.S.P. DOLWEERA, M. JARRELL, University of Cincinnati, TH. MAIER, Oak Ridge National Laboratory, A. MACRIDIN, University of Cincinnati, TH. PRUSCHKE, University of Goettingen, Germany — Using a dynamical cluster quantum Monte Carlo approximation we investigate the d-wave superconducting transition temperature $T_c$ of the doped 2D Hubbard model with a weak inhomogeneity in the form of checkerboard pattern in the hoppings. The hopping within a $2 \times 2$ cluster (plaquette) is $t$ and the hopping between the plaquettes is $t'$ ($0.8t \leq t' \leq t$). We find $T_c$ decreases monotonically with decreasing $t'$ for both fixed $U/t$ or $U/W$ ($U$ the on site Hubbard interaction and $W$ the bandwidth). The characteristic spin excitation energy scale and the strength of d-wave pairing interaction decrease with decreasing $T_c$, suggesting a strong correlation between these two quantities.

3:06PM S11.00004 Electronic properties investigation of YBaCuO using the PAW formalism. SIMON PESANT, MICHEL CÔTÉ, Département de physique et Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — Using density-functional theory (DFT) and the projector-augmented wave (PAW), we characterize the electronic properties of the YBa$_2$Cu$_4$O$_8$-$z$. These systems are metallic or antiferromagnet at room temperature depending on the hole doping induced by oxygen atoms in the basal plane. Also, the impact of an on-site coulomb repulsion term that we don’t know as LDA+$U$, is investigated in the different structures to take into account the highly correlated character of the electrons of those systems. The addition of an on-site coulomb repulsive term does not strongly alter the electronic properties of the YBa$_2$Cu$_4$O$_8$-$z$, and YBa$_2$Cu$_3$O$_{6.5}$ but gives more accurate details about the electronic structure. In the case of YBa$_2$Cu$_3$O$_6$, the impact of the U term is primordial, the anti-ferromagnetism phase being recovered when LDA+$U$ is used, compared to the standard LDA where it is metallic.

3:18PM S11.00005 Electronic properties and chain conductivity of underdoped YBa$_2$Cu$_3$O$_{6+x}$ by First-Principles calculations. VINCENZO FIORENTINI, ALESSIO FILIPPETTI, GIORGIA LOPEZ, MAURO MANTEGA, University of Cagliari, Italy — Metal-insulating transitions in cuprates represent an historical challenge for first-principles calculations. Here we present results obtained through the pseudo-self-interaction free density functional scheme (PSIC) that is capable to correct the gross failures of LSDA at just a moderate increase of computing effort, and works well in both strong-correlated and metallic limit. Here we describe the properties of the end-point systems YBa$_2$Cu$_3$O$_6$ and YBa$_2$Cu$_3$O$_7$ as well as the chemistry of insulating-metal transition occurring in the CuO chains of underdoped YBa$_2$Cu$_3$O$_{6.5}$ in the region $x=0.5$. Coherently with the one-dimensional metallic percolative regime observed at low-doping, we find that the metal-insulating transition occurring at low doping in the non-magnetic Cu(1)Ox chains is induced by chain-like alignment of the doping oxygens within the chains, whereas disorder (i.e. non chain-aligned) distributions are always insulating. In the Cu(2)O$_2$ planes the insulating antiferromagnetic state remains stable up to $x=0.25$, while at $x=0.5$ a normal-metal state, similar to that seen for YBa$_2$Cu$_3$O$_7$, take place. The in-plane antiferromagnetic- paramagnetic competition depends on $x$ but is almost unaffected by the intra-chain order-disorder competition.

3:30PM S11.00006 Holes localization and Fermi Surface morphology of Y$_{1-x}$Ca$_x$BaCu$_3$O$_6$ by First-Principles. GIORGIA LOPEZ, ALESSIO FILIPPETTI, VINCENZO FIORENTINI, University of Cagliari, Italy — The basic chemistry of underdoped Y$_{1-x}$Ca$_x$BaCu$_3$O$_6$ (and of high-$T_c$ superconductors) is permeated by unexplained features. One, in particular, concerns the nature of the non-superconducting phase and its Fermi Surface (FS) whose character is not univocally described by angle-resolved photoemission and Hall measurements, which detect disconnected arcs and pockets, respectively. But what is really missing for a sound interpretation of these data is a robust link between the observed FS and the corresponding electronic structure. As the description of the underdoped regime is hardly accessible through standard First-Principles calculations (FPC), here we use the innovative pseudo-self-interaction corrected local spin density (PSIC) approach to trace an accurate overview of underdoped Y$_{1-x}$Ca$_x$BaCu$_3$O$_6$, with special emphasis on the FS morphology. In particular, the PSIC can predict the formation of Zhang-Rice singlets (ZRS), and we show that electronic states characterized by a mixture of ZRS and antiferromagnetic CuO$_2$ units present, in fact, a variegated series of differently-shaped, disconnected FS that may reconcile the experimental data with a sound interpretation of the underdoped Y$_{1-x}$Ca$_x$BaCu$_3$O$_6$ properties.

3:42PM S11.00007 Nature of high-temperature superconductivity. JOHN D. DOW, Arizona State University, Tempe, AZ 85287-1504 USA, DALE R. HARSHMAN COLLABORATION — Using muon spectroscopy, the high-temperature superconductivity of YBa$_2$(Cu$_2$O$_7$)$_3$ is shown to reside in its BaO layers, not in its cuprate planes. The symmetry of the hole-pairing is s-like, not d-like. The family of superconductors Pb(2)Sr(2)(Y(1-x)R(x))Cu$_3$(O)(3) can be doped p-type (with $R=$Ca) or n-type (with $R=$Ce or Am). The n-type versions do not superconduct, but the p-type compounds do superconduct. The doped ruthenate Ba(2)YRuO(6) begins superconducting in its BaO layers at 92 K. A successful theory of high-temperature superconductivity must explain the ruthenates, the superconducting organic compounds, and the superconducting cuprates. Presently do not.

3:54PM S11.00008 Percolation Theory of the Pseudogap Phase. ALEXEI ABRIKOSOV, Argonne National Laboratory — A concept of the pseudogap state in high-$T_c$ layered cuprates on the basis of percolation theory is proposed. Contrary to the self-consistent BCS critical temperature, which defines $T^*$ - the upper boundary of the pseudogap state, the real critical temperature, $T_c$, is defined, as the percolation threshold, where the infinite cluster appears. This permits to obtain the exact formula for $T_c$, as function of doping and understand its “dome-like” shape.

4:06PM S11.00009 Pairing in Non-Fermi Liquids in Terms of Bethe-Salpeter Equation. YURI MALOZOVSKY, JD Duz Institute for Superconductivity, J.D. FAN, Southern University — The pairing between two fermionic excitations in a non-Fermi liquid is considered in terms of the Bethe-Salpeter equation. We consider the pairing in the Fermi systems with vanishing spectral weight. It is well known that the quasiparticle pole in the single-particle Green’s function in non-Fermi liquids is absent or weak. The examples of such systems can be viewed as the “Marginal” Fermi liquid and Luttinger liquid. Another example that has also been considered is the Fermi system with pseudogap behavior in the spectral weight. Although the pairing between two excitations in non-Fermi liquids is, in general, absent, yet we show that the Cooper’s type pairing can occur and the conditions for such pairing are discussed. The results have also application to the systems with smeared or non-monotonic Fermi distribution. The system that transmits from the Fermi type to Bose type behavior can be a showcase of such systems as discussed.

4:18PM S11.00010 Multiple Pairing in the BCS Model. J.D. FAN, Southern University, YURIY MALOZOVSKY, JD Duz Institute for Superconductivity — We study Cooper’s pairing for more than two particles in terms of the BCS model. We consider the multiple pairing in terms of the BCS Hamiltonian in a quiescent Fermi sea model and in the BCS ground state. Although there is no interaction between Cooper pairs in terms of the BCS Hamiltonian, yet we show that four particles are paired and form a bound state in the singlet state with just twice the bound state energy of a single Cooper’s pair. The four-particle bound state only exists as the result of the Pauli principle and the sharp Fermi edge. We have also shown that the smearing of the Fermi edge due to $\Delta (k)$ as it is in the BCS ground state weakens the pairing of either two or four particles. We show that in the particle-hole channel there exists the multiple particle-hole resonance for four particles and four holes in a quiescent Fermi sea model similar to the case of two particles and two holes resonance. There is no particle-hole resonance in the BCS ground state as shown, which means that the particle-hole resonance is removed by $\Delta (k)$ due to smearing of the Fermi distribution. The wave function for the multiple-pairing model is discussed as well.
4:30PM S11.00011 Extraction of the pairing glue spectra of high Tc superconductors, HAN-YONG CHOI, JAEHYUN YOON, SungKyunKwan Univ, TAKESHI KONDO, ADAM KAMINSKI, Iowa State Univ, CHANDRA VARMA, UC Riverside — We report the current progress of extracting the "pairing glue" spectra of high Tc superconductors. This is done by inverting the d-wave Eliashberg equation, which is an extension of the McMillan-Rowell analysis of the tunneling conductance for conventional s-wave superconductors. A major difference is that there are two distinct \( \alpha^F \) functions for the d-wave superconductors. Consequently, we need twice more experimental inputs to perform this analysis; the pairing function \( \Delta(\omega) \) and self-energy \( \Sigma(\omega) \). This experimental information is currently not available. We therefore first generate \( \Delta(\omega) \) and \( \Sigma(\omega) \) theoretically using the marginal Fermi liquid like glue spectra. Then, using the generated functions as "experimental inputs" we invert the Eliashberg equation to extract the glue spectra. We will compare the input and extracted glue spectra to demonstrate the applicability of the approach. We will next describe how to obtain experimental \( \Delta(\omega) \) and \( \Sigma(\omega) \) from ARPES data. Then, using the obtained experimental inputs we invert the Eliashberg equation to extract the glue spectra. The results will be reported for several temperatures above and below Tc.

4:42PM S11.00012 A competing order scenario of two-gap behavior in hole doped cuprates, TAMNOY DAS, R.S. MARKIEWICZ, A. BANSIL, Northeastern University — Angle-dependent studies of the gap function provide evidence for the coexistence of two distinct gap modes in hole doped cuprates, where the gap near the nodal direction scales with the superconducting transition temperature \( T_c \), while that in the antinodal direction scales with the pseudogap temperature. We present model calculations[1] which show that most of the characteristic features observed in the recent angle-resolved photoemission (ARPES) as well as scanning tunneling microscopy (STM) two-gap studies are consistent with a scenario in which the pseudogap has a non-superconducting origin in a competing phase. Our analysis indicates that, near optimal doping, superconductivity can quench the competing order at low temperatures, and that some of the key differences observed between the STM and ARPES results can give insight into the superlattice symmetry of the competing order. Work is supported in part by the USDOE.


4:54PM S11.00013 Local quasiparticle lifetimes in a d-wave superconductor, S. GRASER, P.J. HIRSCHFELD, Physics Department, University of Florida, Gainesville, FL 32611 USA, D.J. SCALAPINO, Department of Physics, University of California, Santa Barbara, CA 93106-9530 USA — Recently, scanning tunneling spectroscopy (STS) measurements have exhibited good fits to conductance spectra at the surface of Bi-2212 using a BCS-type model for a d-wave superconductor and assuming a local quasiparticle scattering rate varying linearly with energy. Employing a model of quasiparticle scattering by impurities and spin fluctuations we argue that the broadening of the local density of states is in general given by the self-energy of the system averaged over a small region. The size of this region at low energies is shown to be significantly larger than a gap "patch", a region over which the gap is roughly constant in this system; states measured by STS are therefore very homogeneous in this energy range. At energies above a scale determined by disorder, STS averages over states localized within a gap "patch", and lifetimes are correspondingly inhomogeneous. We show that the local self-energy in the impurity-plus-spin fluctuation model can explain the data as well as the phenomenological linear scattering rate extracted from experiment.

5:06PM S11.00014 Disordered superconductors: role of interaction strength, RAIMUNDO DOS SANTOS, FELIPE MONDAINI, THEREZEA PAIVA, Universidade Federal do Rio de Janeiro, RICHARD SCALETTER, UC-Davis — We have considered the half-filled disordered attractive Hubbard model, in which the on-site attraction is switched off on a fraction \( f \) of sites, while keeping a finite \( U \) on the remaining ones. The configurationally-averaged equal-time pair structure factor has been calculated as a function of temperature, through Quantum Monte Carlo simulations for several \( f \) and \( U \), and a finite-size scaling ansatz has been used for the zero-temperature gap. We have found that the system sustains superconductivity in the ground state up to a critical impurity concentration, \( f_c \), which increases with \( U \) at least up to the largest values of \( U \) we have considered. Also, the normalized zero-temperature gap as a function of \( f \), for fixed \( U \), shows a maximum near \( f_{\text{max}} \), within a range of \( U \) values, thus indicating that a small amount of disorder can initially enhance superconductivity. We argue that, overall, the observed behavior results from both the breakdown of CDW-superconductivity degeneracy and the fact that free sites tend to "push" electrons towards attractive sites.

5:18PM S11.00015 A singlet-pairing superconductor is always also a super-spin-current-conductor, CHIA-REN HU, Texas A&M University — A heuristic argument and a simple theory are used to show that, as a fundamental difference between BEC and BCS condensation of fermion pairs, the later, even for singlet pairing, can carry a sizable dissipation-less spin-current below practically the same \( T_c \). The heuristic argument is based on the similarity between a spin-current carried by a singlet-pairing condensate and (coherent) partner changing in a dancing hall. Simple theory: We consider singlet pairing in a normal metal carrying a moderate spin-current, which causes the spin-up- and -down Fermi surfaces (FSs) to be shifted in the momentum space by \( \pm q/2 \). \( (k,\uparrow),(k,\downarrow) \)-pairing is clearly still possible over the entire FSs. To favor a spin current in the system, we introduce a vector Lagrange multiplier \( \omega_{sp} \), and add \(-\omega_{sp} \sum_{k}\sigma h c_{k,\sigma}c_{-k,\sigma} \) to the Hamiltonian. Since time-reversal invariance is not broken, negligible changes to all properties of the singlet-pairing state follow, and the system remains fully gapped. No depairing can be induced even for a sizable spin current. Two experimental tests of this prediction will be discussed.

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S12 DCMP: Strongly Correlated Quantum Phases
Morial Convention Center 203

2:30PM S12.00001 Fate of the Fermionic Quasiparticles at the Electronic Nematic-Smectic Quantum Critical Point, KAI SUN, BENJAMIN FREGOSO, EDUARDO FRADKIN, UIUC — We use the order-parameter theory of the electronic nematic-smectic critical transition of the fermionic liquid crystal phases, discussed in the previous talk, to study the effect of the low energy bosonic modes on the fermionic quasiparticles using RPA. Both the continuous model, which has a continuous rotational symmetry, and the lattice model, which has a discrete point group symmetry are studied. We find that at the nematic-smectic critical point, due to the critical smectic fluctuations, the dynamics of the fermionic quasiparticles near several points on the Fermi surface, which eventually become gapped under the development of CDW order, are not governed by a Landau Fermi liquid. Surprisingly, the fermions in the smectic phase also form a non-Fermi liquid. The transition between the quantum liquid crystal phases and the insulating CDW state is also discussed.
previous studies. The presence of a phase exhibiting both the plaquette and the columnar properties. This also presents a natural framework for resolving the disagreement between local constraint. By combining an analysis of the excitation gaps of different symmetry sectors with information on plaquette structure factors, we show the in the context of high-temperature superconductivity, and its descendants have taken on a central role in the study of quantum systems incorporating a hard charge density wave order, and construct an order-parameter theory. Its static part has the McMillan-DeGennes form of the classical smectic-nematic phase transition, while its quantum dynamics is dominated by the coupling to the electronic quasiparticles. Both, commensurate and incommensurate cases are studied. The spectrum of the nematic phase has low energy "fluctuating stripes". We also provide evidence that, contrary to the classical case, the gauge-type of coupling between the nematic and smectic at the critical point is irrelevant at this QCP. We discuss the relevance of these ideas to the phenomenology of the high $T_c$ superconductors. [1] S. A. Kivelson, E. Fradkin and V. J. Emery, nature 393, 550, 1998.

3:06PM S12.0004 Universal Scaling in the Fan of an Unconventional Quantum Critical Point, ROGER MELKO, University of Waterloo, RIBHU KAUL, Harvard University — We present the results of stochastic series expansion Quantum Monte Carlo simulations on a 2D S=1/2 Heisenberg model with additional four-spin interaction — the so-called ‘JQ’ model [1]. Using extensive simulations on lattice sizes containing in excess of $10^4$ spins, we examine the claim that the observed Néel to valence-bond-solid (VBS) quantum phase transition is consistent with the ‘deconfined’ quantum criticality scenario. We discuss finite-temperature properties of the conjectured quantum critical fan [2], including scaling behavior, the calculation of universal critical exponents, and the apparent emergence of a global U(1) symmetry in the VBS order parameter. Finally, we consider several extensions of the model that may help give further insight into the nature of this unconventional quantum phase transition.


3:18PM S12.0005 Quantum critical scaling behavior of deconfined spinons, FLAVIO NOGUEIRA, Institute for Theoretical Physics, Free University Berlin and Ames Laboratory, STEINAR KRAGSET, ASLE SUDBO, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway — The quantum scaling behavior of deconfined spinons for a class of field theoretic models of quantum antiferromagnets is considered. The competition between the hedgehogs and the Berry phases is discussed from a renormalization group perspective. An important result following from our analysis is the computation of the anomalous dimension for the decay of spin correlations. Our results confirm the expectation that the transition from a Néel to a valence-bond solid state belongs to a completely new universality class.

3:30PM S12.0006 Monte-Carlo simulations of su(2) symmetric deconfined criticality action, A.B. KUKLOV, CSI, CUNY, M. MATSUMOTO, Universite Paul Sabatier, Toulouse ; ETH Zurich, N.V. PROKOF’EV, UMASS, Amherst; ETH Zurich; Kurchatov Institute, Moscow, B.V. SVISTUNOV, UMASS, Amherst; ETH Zurich; Kurchatov Institute, Moscow, M. TROYER, ETH Zurich — We discuss results of Monte Carlo simulations of su(2) symmetric deconfined criticality action in $CP^1$ formulation proposed by T. Senthil, et. al, Science 303, 1490 (2004). Using high-temperature expansion we reformulate the partition function in terms of J-currents. The resulting configuration space is explicitly su(2) symmetric. Critical behavior in the region of possible deconfined critical point (DCP) is addressed by the flow method [A.B.Kuklov, et.al., Annals of Physics 321,1602(2006)] mapping critical properties of a system with small values of the gauge interaction $g$ at large sizes to a system with large $g$ and small sizes. We observe data collapse on a single master curve with the flow toward fluctuation induced I order transition. The unlikely possibility of existence of the lower tricritical point separating I order transitions from the DCP line is assessed in terms of disruption of the flow collapse.

3:42PM S12.0007 Phase diagram of the anisotropic two-dimensional bilinear biquadratic spin-1 Heisenberg model, CHRISTOPH PUETTTER, MICHAEL LAWLER, HAE-YOUNG KEE, Department of Physics, University of Toronto, Toronto, Canada M5S 1A7 — The anisotropic bilinear biquadratic Heisenberg model on a square lattice has been proposed to exhibit deconfined critical phenomena (DCP) based on QMC simulations and effective field theoretical studies [1, 2]. We investigate the phase transitions of the model using slave boson representation. Our mean field approach suggests a first order transition between the nematic and the disordered regime except at the tricritical SU(3) symmetric point. We will also discuss the relevance of our results to the DCP.


3:54PM S12.0008 Generic mixed columnar-plaque phases in Rokhsar-Kivelson models, RALKO ARNAUD, POILBLANC DIDIER, LPT - University of Toulouse, France, MOESSNER RODERICH, MPI-PKS, Dresden, Germany — We revisit the phase diagram of Rokhsar-Kivelson models, which are used in fields such as superconductivity, frustrated magnetism, cold bosons, and the physics of Josephson junction arrays. From an extended height effective theory, two simple generic phase diagrams are obtained. The first one is a first order transition scenario between the columnar and the plaquette phases, common in such models. The second, more exotic, exhibits a second order transition and contains a mixed phase that interpolates continuously between columnar and plaquette states. From exact diagonalization and Green’s function Monte Carlo techniques, we present evidence that a realization of the latter scenario occurs in the Rokhsar-Kivelson square lattice Quantum Dimer model. This model, originally proposed in the context of high-temperature superconductivity, and its descendants have taken on a central role in the study of quantum systems incorporating a hard local constraint. By combining an analysis of the excitation gaps of different symmetry sectors with information on plaquette structure factors, we show the presence of a phase exhibiting both the plaquette and the columnar properties. This also presents a natural framework for resolving the disagreement between previous studies.
4:06PM S12.00009 An exact chiral spin liquid with non-Abelian anyons, HONG YAO, STEVEN KIVELSON, Department of Physics, Stanford University — We establish the existence of a “chiral spin liquid” (CSL) as the exact ground state of the Kitaev model on a decorated honeycomb lattice, which is obtained by replacing each site in the familiar honeycomb lattice with a triangle [1]. This state spontaneously breaks time reversal symmetry but preserves other symmetries. There are two topologically distinct CSL’s separated by a quantum critical point. Interestingly, vortex excitations in the topologically nontrivial CSL (Chern number \( \pm 1 \)) obey non-Abelian statistics.


4:18PM S12.00010 Non-abelian topological phases and unconventional criticality in a model of interacting anyons, CHARLOTTE GILS, ETH Zurich, SIMON TREBST, Microsoft Research, Station Q, MATTHIAS TROYER, ETH Zurich, ANDREAS LUDWIG, UC Santa Barbara, ALEXEI KITAEV, Caltech — Non-abelian topological phases have recently attracted considerable interest in the context of fault-tolerant quantum computation. However, such phases have only been established in a small set of microscopic models, one of which involves interacting spin-1/2 degrees of freedom on a honeycomb lattice (Levin, Wen 2005). In particular, this model supports quasiparticle excitations that can be described as so-called Fibonacci anyons. We have reformulated this model in terms of anyonic degrees of freedom and consider the case of interacting anyonic quasiparticles by adding a magnetic field term to the Hamiltonian. Our analysis of a quasi-one-dimensional ladder model not only shows the (extended) stability of the topological phase when perturbed by such local terms, but also demonstrates the role of topology in determining the exact nature of these phases. Interestingly, the magnetic field can drive a phase transition between two distinct topological phases. Numerically, we establish that this critical point can be described by a conformal field theory with central charge \( c = 14/15 \). This observation has lead to an analytical understanding of this critical point which can be mapped to an exactly solvable transfer matrix representation in terms of a restricted-solid-on-solid (RSOS) model.

4:30PM S12.00011 Topological Mott Insulators, CHARLOTTE GILS, ETH Zurich, SIMON TREBST, Microsoft Research, Station Q, MATTHIAS TROYER, ETH Zurich, ANDREAS LUDWIG, UC Santa Barbara, ALEXEI KITAEV, Caltech — Non-abelian topological phases have recently attracted considerable interest in the context of fault-tolerant quantum computation. However, such phases have only been established in a small set of microscopic models, one of which involves interacting spin-1/2 degrees of freedom on a honeycomb lattice (Levin, Wen 2005). In particular, this model supports quasiparticle excitations that can be described as so-called Fibonacci anyons. We have reformulated this model in terms of anyonic degrees of freedom and consider the case of interacting anyonic quasiparticles by adding a magnetic field term to the Hamiltonian. Our analysis of a quasi-one-dimensional ladder model not only shows the (extended) stability of the topological phase when perturbed by such local terms, but also demonstrates the role of topology in determining the exact nature of these phases. Interestingly, the magnetic field can drive a phase transition between two distinct topological phases. Numerically, we establish that this critical point can be described by a conformal field theory with central charge \( c = 14/15 \). This observation has lead to an analytical understanding of this critical point which can be mapped to an exactly solvable transfer matrix representation in terms of a restricted-solid-on-solid (RSOS) model.

4:42PM S12.00012 Critical liquid phases for frustrated bosons in two dimensions, OLEXEY MOTRUNICH, California Institute of Technology, MATTHEW P.A. FISHER, Microsoft Corporation, Station Q, University of California Santa Barbara — An interesting question in strongly correlated systems is the possibility of a “metallic” bosonic liquid — a quantum liquid phase of bosons that is neither superfluid nor Mott insulator. We present an attempt to construct such states using slave particle technique borrowed from theories of spin liquids; the approach can be also be taken as a flux attachment treatment performed in the absence of time reversal breaking. We describe properties of such constructed boson liquid states, which support gapless boson excitations residing on “Bose surfaces” in the momentum space and exhibit power law correlations in various properties. We also suggest a promising model Hamiltonian of hard-core bosons hopping on a square lattice and with frustrating ring exchanges which may have such a phase.

4:54PM S12.00013 Pseudogap in strongly interacting and strongly disordered systems, SIMONE CHIESA, PRA Buddha CHAKRABORTY, WARREN PICKETT, RICHARD SCALETTAR, UC Davis — The interplay of disorder and correlation is known to give rise to anomalies in the density of states at the chemical potential of quantum and classical systems. In particular, in the quantum case, the diagrammatic calculation of Altschuler and Anson predicts a pseudo-gap for the case of a weakly disordered and weakly interacting metal. Here we report a numerical study suggesting that such anomalies are present also in the case of strongly interacting and strongly disordered systems. We consider the Hubbard model in the presence of diagonal disorder and diagonalize small clusters (up to 12 sites) in the framework of a grand canonical scheme involving twisting the boundary condition. For a given interaction and disorder strength we observe the formation of a pseudo-gap whose shape and depth is largely insensitive to the particle density. For a given particle density the pseudo-gap gets deeper as the interaction and the disorder are increased.

5:06PM S12.00014 Bose Metal Phase from Inhomogeneous Flow, GERGELY ZIMANYI, Physics Department, UC Davis, NIELS JENSEN, Department of Applied Science, UC Davis — Numerous experiments report a Bose Metal phase between the Superconducting (S) and the Insulating (I) phases at an SI transition. [1,2] However, theoretically the origin of the corresponding dissipation remains unclear. We propose a picture in which inhomogeneous superconducting flow occurs in channels/filaments, defined by islands of localized Bose Glass. The superconducting bosons interact with the localized bosons of the Bose Glass via the Coulomb interaction. This Coulomb drag generates an effective dissipation for the superflow. We developed a new numerical technique to simulate superconductivity by inertial dynamics and a current generator. We found a Bose Metal phase in a finite range of the disorder, bracketed by the superconducting and insulating phases. The noise spectrum was also determined and compared to recent experiments. [1] H.M. Jaeger, D.B. Haviland, B.G. Orr and A.M. Goldman, Phys. Rev. B 40, 182 (1989). [2] A. Yazdani and A. Kapitulnik, Phys. Rev. Lett. 74, 3037 (1995); M. Steiner, N. Breznay and A. Kapitulnik, arxiv: 0710.1822.

5:18PM S12.00015 Double Occupancy in low-energy theories of doped Mott insulators, PHILIP PHILLIPS, TING PONG CHOY, ROBERT LEIGH, University of Illinois, GEORGE SAWATZKY, University of British Columbia — We review how a proper low-energy theory can be constructed for the Hubbard model by explicitly integrating over the degrees of freedom far away from the chemical potential. A surprising feature of the exact low-energy theory is the emergence of an elementary charge 2e boson which mediates double occupancy much below the Mott scale. We show that within the standard canonical transformation formalism to derive the \( t - J \) model from the Hubbard model, a similar feature (double occupancy below the Mott scale) appears only if the electron creation and annihilation operators are properly transformed as well. By comparing precisely how the electron operators transform in both theories, we are able to show that the charge 2e boson mediates dynamical spectral weight transfer across the Mott gap. At half-filling, the interactions mediated by the charge 2e boson defeat the artificial local SU(2) symmetry found earlier in the projected \( t - J \) model. R. G. Leigh, P. Phillips and T. -P. Choy, Phys. Rev. Lett. 99 46404 (2007); arxiv:07071554 (PRB, in press).

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S13 DCOMP DCP: Focus Session: Frontiers in Electronic Structure Theory I – Morial Convention Center 204
H. J. Kulik, M. Cococcioni, D. Scherlis and N. Marzari, PRL thus fruitfully employ GGA+U in the study of large-scale complexes which contain hundreds of atoms such as the active site of halogenating enzymes and will further highlight how our method affords substantial improvement in the physical description of hybridization and bonding irrespective of system size. We + approximation (GGA) with a Hubbard U which is obtained from a self-consistent linear response procedure can greatly improve the description of both spin state

Q.-M. Hu, K. Reuter, and M. Scheffler, PRL adsorption energetics from present-day DFT xc functionals with hybrid functional and Møller-Plesset perturbation theory calculations for small clusters. From untractable with correlated wave function techniques. We overcome these limitations with a recently introduced “local xc correction” scheme [1], correcting the is uncertain to properly account for this type of bonding, while the system sizes required to correctly grasp the metallic band structure are computationally severe challenge for accurate first-principles calculations. Density-Functional Theory (DFT) with local and semi-local exchange-correlation (xc) functionals a local exchange-correlation correction scheme

HEATHER KULIK, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Despite the importance of transition metal centers in a variety of biological and inorganic chemical reactions, density functional theory calculations often fail quantitatively in describing both the stable intermediate electronic structures, splittings, and geometries as well as reaction barriers and geometries of transition states. We have shown that augmenting the generalized-gradient approximation (GGA) with a Hubbard U which is obtained from a self-consistent linear response procedure can greatly improve the description of both spin state splittings in the iron dimer as well as reaction barriers in the addition-elimination reaction of hydrogen and methane with FeO+2. This fully ab-initio GGA+U approach provides excellent agreement with accurate, correlated-electron quantum chemistry calculations but at a fraction of the cost of these methods. We will further highlight how our method affords substantial improvement in the physical description of hybridization and bonding irrespective of system size. We thus fruitfully employ GGA+U in the study of large-scale complexes which contain hundreds of atoms such as the active site of halogenating enzymes and various porphyrin complexes.

HEATHER KULIK, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Despite the importance of transition metal centers in a variety of biological and inorganic chemical reactions, density functional theory calculations often fail quantitatively in describing both the stable intermediate electronic structures, splittings, and geometries as well as reaction barriers and geometries of transition states. We have shown that augmenting the generalized-gradient approximation (GGA) with a Hubbard U which is obtained from a self-consistent linear response procedure can greatly improve the description of both spin state splittings in the iron dimer as well as reaction barriers in the addition-elimination reaction of hydrogen and methane with FeO+2. This fully ab-initio GGA+U approach provides excellent agreement with accurate, correlated-electron quantum chemistry calculations but at a fraction of the cost of these methods. We will further highlight how our method affords substantial improvement in the physical description of hybridization and bonding irrespective of system size. We thus fruitfully employ GGA+U in the study of large-scale complexes which contain hundreds of atoms such as the active site of halogenating enzymes and various porphyrin complexes.

For molecules, the resulting numerical effort usually restricts these methods to Gaussian basis functions. We here show how all these methods can be handled accurately with efficient all-electron numerical atom-centered basis sets [1] by using a second, auxiliary basis for products of basis functions (resolution of the identity). For an extended set of finite systems spanning small molecules (water dimer, benzene), metal clusters (Na, ) and biomolecules (polyalanine peptides), we demonstrate that the efficiency of optimized numeric atom-centered basis sets is directly carried over into our new approach. Our approach is then applied to analyze the CO-adsorption problem (CO/Cu(111)). [1] V. Blum et al., The FHI-aims project, www.fhi-berlin.mpg.de/aims

2:42PM S13.00002 Order N Implementation of Exact Exchange XIFAN WU, Princeton University, ANNABELLA SELLONI, ROBERTO CAR — Exact (Hartree Fock) exchange is needed to overcome some of the limitations of local and semilocal approximations of density functional theory (DFT). Moreover exact exchange is a basic ingredient in modern approaches to compute excitation properties, like the GW and the OEP schemes. So far, however, computational cost has limited the use of exact exchange in plane wave calculations for extended systems. We show that this difficulty can be overcome by performing a unitary transformation from Bloch to Maximally Localized Wannier functions in combination with an efficient technique to compute real space Coulomb integrals. The resulting scheme scales linearly with system size and, when used in ab-initio molecular dynamics simulations, requires only a modest increase in computational cost compared to standard DFT implementations. We validate the scheme with representative applications.
4:06PM S13.00007 Transcorrelated method applied to covalent and ionic solids: total energy and band structure calculation. KEITARO SODEYAMA, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo, REI SAKUMA, JST-CREST, AIST — To calculate the electronic structures of solids including correlation effects, we have developed the transcorrelated (TC) method, which was first proposed by Boys and Handy. In the TC method, the wave function is represented by a correlated wave function \( \Phi \), where \( \Phi \) is a single Slater determinant and \( F \) is a Jastrow function, \( F = \exp[-\sum_{i<j} u_{ij}] \), \( u_{ij} \) is a two-body function called Jastrow factor. The many-body Hamiltonian \( \hat{H} \) is similarity transformed to an effective Hamiltonian \( \hat{H}_{TC} = F^{-1} \hat{H} F \) with up-to-three-body interaction. One-electron orbitals and their orbital energies are optimized by solving a set of Hartree-Fock (HF)-like single particle equations derived by minimizing the variance of the \( \hat{H}_{TC} \). In this study, the band gaps and total energies of covalent and ionic solids were calculated by the TC method at various lattice constants. The local density approximation (LDA) and HF calculations were also performed to the same systems and compared to the TC results. In covalent solids such as silicon carbide, the lattice constant and bulk modulus calculated by the TC method were not largely different from the LDA results. In ionic solids such as lithium hydride, we found that the lattice constant, bulk modulus and band gap calculated by the TC method were closer to the experimental results than the LDA results.

4:18PM S13.00008 System-averaged exchange and correlation holes in third-row atoms. ANTONIO C. CANGIO, Ball State University — Recent work is presented on the theoretical calculation of system-averaged exchange and correlation holes (intracules) for a pseudopotential model of the valence shell of third-row atoms. Exchange holes are obtained from numerical fourier transform methods and correlation holes from variational quantum Monte Carlo calculations using the method of correlated estimates. We observe approximate scaling behavior in both exchange and correlation, following the known scaling of the valence density across the row. The holes are compared to density-functional models including LDA, GGA and meta-GGA approaches. Particular attention is paid to self interaction (SI) error; we find that a sizeable error occurs in the same-spin channel of the correlation hole which persists for the LDA and GGA even after standard SI corrections are applied. A simple SI correction that eliminates this error will be discussed.

4:30PM S13.00009 RPA Correlation Energy in ACFD Formalism with Thomas-Fermi-von Weizsäcker Approximation. VIET HUY NGUYEN, STEFANO DE GIRONCOLI, Intnl School for Adv Studies (SISSA), Trieste Italy — It is well known that LDA or GGAs approximations in DFT do not describe correctly systems where long range correlations are important. In the Adiabatic Connection Formalization-Dependence (ACFD) formalism correlation energy can be computed exactly from Kohn-Sham and interacting linear response functions. Although computationally very demanding, this formalism has shown to describe correctly systems where standard DFT fails qualitatively by combining RPA xc-kernel with short-range local-density corrections (RPA+). On the other hand, Thomas-Fermi-von Weizsäcker approximate kinetic response function can capture reasonably well asymptotic long range interactions via van der Waals coefficients, and has the computationally desirable feature that it only involves a single auxiliary wavefunction regardless of the number of electrons in the system. Here, we show how to use this approach to calculate approximate RPA correlation energies. Numerical results for atoms show that this approach gives approximate RPA correlation energies closer to the experimental values than those obtained by full RPA and, when combined with a short-range local-density correction, it gives results at least as good as those of full RPA+. The possibility is therefore open to address large systems where correlations need to be treated beyond LDA and GGAs.

4:42PM S13.00010 Generalized density functional theory for effective potentials in many-body electronic structure. F. A. REBOREDO, P. R. C. KENT, Oak Ridge National Laboratory — We demonstrate the existence of different density functionals that retain selected properties of the many-body ground state in the non-interacting density functional solution. We focus on diffusion Monte Carlo applications that require trial wave functions with Fermion optimal nodes. The theory can be extended and used to understand current practices in several electronic structure methods [GW-BSE,CLEPM] within a generalized density functional framework. The theory justifies and stimulates the search of optimal empirical density functionals and effective potentials but also cautions on the limits of their applicability. The theoretical concepts are tested against a near-analytic model that can be solved to numerical precision. Research performed at the Materials Science and Technology Division and the Center of Nanophase Material Sciences at Oak Ridge National Laboratory sponsored the Division of Materials Sciences and the Division of Scientific User Facilities U.S. Department of Energy.

5:06PM S13.00011 Real or artifactual symmetry breaking in BNB: A fixed-node diffusion Monte Carlo study1, WISSAM A. AL-SAIDI, CYRUS UMRIGAR, Cornell University — The linear BNB molecule represents one of the most challenging examples of symmetry-breaking effects because of its susceptibility to a second-order Jahn-Teller distortion along the antisymmetric stretching mode. This real symmetry breaking could be confused in calculations with an artifactual one caused by the approximate nature of the theoretical approach. Thus the debate of whether the ground state of BNB is symmetric in the positions of the boron atoms with respect to nitrogen or if this symmetry is broken. Our preliminary investigations with diffusion Monte Carlo shows that the symmetric and the broken symmetry geometries are nearly degenerate, which would suggest a highly floppy quasi-symmetric BNB ground state.

5:18PM S13.00012 Potential Energy Curves and Excited States of the C2 Molecule by Auxiliary-Field Quantum Monte Carlo (AFQMC)1, WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary, WISSAM AL-SAIDI, Cornell University — The accurate determination of potential energy curves (PECs) and excited states represents two difficult problems in electronic structure calculations. We present AFQMC PECs of the challenging C2 molecule, focusing on the ground state and two singlet low-lying excited states. AFQMC calculates a target many-body wave function (WF) by means of random walks in the space of Slater determinants. We employ truncated complete active space (CAS) trial WFs (\( \Psi_j \)) to guide the AFQMC projection to obtain the desired state. With the phase-free constraint, the CAS \( \Psi_j \) is effective in controlling the sign/phase problem, and filtering in the desired excited state. The AFQMC results are in very good agreement with exact results and in comparison with experimental spectroscopic constants will also be presented.

1Supported by NSF and DOE.

1Supported by DOE CMSN, ONR, NSF, and ARO. Calculations were performed at the CPD and W&M SciClone.

2:30PM S14.00001 Strongly interacting Fermi gases in an optical lattice. NIELS STROHMÄIER, ROBERT JOERDENS, ETH Zurich, KENNETH GUENTER, Ecole Normale Superieure, Paris, YOSUKE TAKASHI, Kyoto University, MICHAEL KOEHL, University of Cambridge, HENNING MORITZ, TILMAN ESSLINGER, ETH Zurich — When cold fermionic atoms are placed in the periodic potential of an optical lattice, they behave similarly to electrons in a crystal. However, the properties of this synthetic material can be changed at will. Here, we report on the experimental realization and investigation of strongly interacting Fermi gases with tunable interactions. By changing the interaction strength we are able to control the transport properties: while dipole oscillations are observed for a non-interacting gas, the atomic cloud relaxes very slowly to its equilibrium position for strong attractive interactions. We suggest an interpretation in the framework of the Hubbard model including external confinement: local fermionic pairing occurs, leading to a drastically reduced tunneling rate. Furthermore, experimental results on the behavior of repulsively interacting Fermi gases will be presented.

2:42PM S14.00002 Squeeing out the entropy of Fermions in an optical lattice. QI ZHOU, TIN-LUN HO, Physics Department, The Ohio State University, Columbus, OH, 43210 — We point out a new scheme for achieving the strongly correlated system in an optical lattice. By turning the bulk of the trapped fermions into a band insulator, the entropy of the system is expelled to the surface and removed by various means. Our scheme also illustrates a general principle of cooling in a many body system. That is, one can use a gapped state to squeeze out the entropy and then turn it into the desired state after the entropy is removed.

2:54PM S14.00003 Superfluid-insulator transitions of the Fermi gas with near-unitary interactions in a periodic potential. EUN-GOOK MOON, Harvard University, PREDRAG NIKOLIC, Rice University, SUBIR SACHDEV, Harvard University — We consider a gas of spin-1/2 fermions with interactions near the unitary limit. In an applied periodic potential, and with a density of an even integer number of fermions per unit cell, there is a second-order quantum phase transition between superfluid and insulating ground states at a critical amplitude of the lattice potential. We map out the universal phase diagrams at $N = \infty$ in a model with Sp(2N) spin symmetry, and compute the universal ratio between the critical lattice amplitude and molecule recoil energy. As the interactions between fermions are varied, the insulator evolves smoothly between a band insulator of fermions and a Mott insulator of fermion pairs. We discuss implications for recent ultra-cold atom experiments.

3:06PM S14.00004 Pattern formation in mixtures of different mass ultracold atoms in optical lattices: an inhomogeneous DMFT study. JAMES FREERICKS, Department of Physics, Georgetown University — Dynamical mean-field theory (DMFT) is generalized to include an inhomogeneous trap and applied to the problem of different mass spin-polarized fermionic atoms that have an interspecies interaction $U$. Such a system is described by the spinless Falicov-Kimball model in a harmonic trap (in the limit where the more massive atom is localized on the optical lattice); we examine atoms moving on a 51X51 two-dimensional square lattice. When the temperature is low enough, the system exhibits pattern formation with different types of order, ranging from checkerboard phases and phase separation to an analog of the viscous fingering seen in immiscible liquids. The temperature evolution of these ordered phases is interesting as well, as the system can form rings of ordered phases surrounding disordered phases, which expand in size as $T$ is lowered. These patterns can be detected with noise-correlation spectroscopy or Bragg scattering, and their evolution with $T$ could be employed for thermometry. The inhomogeneous DMFT algorithm parallels well and is quite efficient. The main difference with exact numerical solutions or the local density approximation is that the temperature scales for the ordering are significantly higher in the IDMFT solution.

3:18PM S14.00005 Fermion mixtures on an optical lattice. SHAN-WEN TSAI, University of California, Riverside, TUN WANG, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences — We investigate mixtures of two species of fermionic ultracold atoms loaded on an optical lattice. We consider fermions with unequal masses and also fermions with unequal spin populations. We discretize the two Fermi surfaces and employ a functional renormalization-group (RG) approach to calculate the flows of effective interaction vertices in order to identify the instabilities of the system. Without any interactions produced via tuning of Feshbach resonances, a question arises as to whether there can be BCS pairing from repulsive interactions (produced by the optical trap) combined with lattice effects. For spin-independent bare contact interaction, the RG flows for unequal spin populations generate effective spin-dependent interactions. We investigate cases with different interactions, both attractive and repulsive, and different shapes of the Fermi surfaces, in particular the case when one of the fermion species has a nested Fermi surface and the other one does not.

3:30PM S14.00006 Effects of frozen double occupancies in fermions in optical lattices. RAJDEEP SENARMU, EUGENE DEMLER, Harvard University, EHUD ALTMAN, Weizmann Institute — We study the effects of “frozen” double occupancies in metastable states of 3D fermionic Hubbard model in the strongly interacting regime. Such long lived states can be created with ultracold fermions in an optical lattice, as the lattice potential is ramped up to access strongly correlated regimes. We shall discuss how the presence of the double occupancies affect anti-ferromagnetism in these systems. We will also discuss possible “charge” orders in these systems.

3:42PM S14.00007 Dynamical instabilities of paired fermion superfluids in optical lattices. GANESH RAMACHANDRAN, University of Toronto, ANTON BURKOV, University of Waterloo, ARUN PARAMEKTANTI, University of Toronto — We report on a study of dynamical instabilities in cold atom fermionic superfluids in optical lattices. Of particular interest to us are the properties of such superfluids at fermion densities corresponding to noninteger average number of pairs per lattice site. In this case superfluidity competes with charge-density-wave ordered states, which has a profound effect on how such superfluids respond to flow. In particular, by varying the pairing momentum, we find a complex interplay between dynamical, pair breaking and Landau (phonon excitation) instabilities at different fillings and different magnitudes of the pairing interaction. Using insights from this study, we construct the “dynamical phase diagrams” of fermion superfluids, and discuss the experimental observability of the proposed effects.

3:54PM S14.00008 BCS-BEC Crossover of a Quasi-two-dimensional Fermi Gas: the Significance of Dressed Molecules. WEI ZHANG, GUIN-DAR LIN, LUMING DUAN, Department of Physics, University of Michigan — We study the crossover of a quasi-two-dimensional Fermi gas trapped in the radial plane from the Bardeen-Cooper-Schrieffer (BCS) regime to the Bose-Einstein condensation (BEC) regime by crossing a Feshbach resonance. Using an effective two-dimensional Hamiltonian with renormalized interaction between atoms and dressed molecules, we calculate the zero temperature cloud size and number density distribution and conclude that the results are consistent with the picture of BCS-BEC crossover. These results are in clear contrast to the predictions of an effective two-dimensional Hamiltonian with renormalized atom-atom interaction, where a constant cloud size and identical density profile are expected for arbitrary detunings. This inconsistency indicates that the inclusion of dressed molecules is essential to describe the two-dimensional Fermi systems, especially on the BEC side of the Feshbach resonance. 

Wednesday, March 12, 2008 2:30PM - 5:18PM — Session S14 DAMOP: Fermions in Optical Lattices Morial Convention Center 205

Supported by DARPA under grant number W911NF-07-1-0576.

Supported by NSF and Samsung Scholarship.
4:06PM S14.00009 Itinerant Ferromagnetism in an Atom Trap

ILYA BERDKIKOV, PIERS COLEMAN, Center for Materials Theory, Rutgers University, STEVE SIMON, Bell Labs, Alcatel-Lucent — Interest in ferromagnetism has prompted the development of many theoretical techniques to study the phenomenon. However, even the most sophisticated schemes, though well motivated physically, remain intrinsically uncontrolled. This is a clear signal that more experimental input is needed, and the rapidly developing field of ultra-cold atomic gases affords just such an investigation. We propose an experiment to explore the magnetic phase transition in interacting fermionic systems, and establish signatures of ferromagnetic correlations in the observed ground states. We find, that for large trap radii \( R > l \), in units of coherence length \( \xi \), ground states are topological in nature, a “skyrmion” in 2D, and a “hedgehog” in 3D. Finally, we describe how to obtain the ferromagnetic phase diagram of itinerant electron systems from these experiments.

4:18PM S14.00010 The expansion of strongly interacting fermions after the release from a trap

FABIAN HEIDRICH-MEISNER, Institut fuer Theoretische Physik C, RWTH Aachen, Germany, MARCOS RIGOL, Department of Physics, University of California, Santa Cruz, CA, USA, ALEJANDRO MURAMATSUMU, Institut fuer Theoretische Physik III, Universitaet Stuttgart, Germany, ADRIAN FEIGJUN, Microsoft Q, University of California, Santa Barbara, CA, USA, ELBIO DAGOTTO, Materials Science and Technology Division, ORNL, and University of Tennessee, Knoxville, TN, USA — Both the recent experimental progress in cold atom gas realizations and developments in computational techniques has fueled interest in nonequilibrium properties of strongly correlated systems. Here we study the expansion of fermions in a one-dimensional lattice after released from a trap. Using the time-dependent density matrix renormalization group method, we analyze properties of the one-particle density matrix as well as the evolution of spin and density correlations. A comparison of particles escaping from a metallic region as compared to a Mott-insulating one shows that some memory on the initial state is preserved during the expansion. We further address the question to what extent the correlations measured during the expansion and thus in a non-equilibrium situation resemble those of appropriately chosen reference systems in equilibrium.

4:30PM S14.00011 Quantum Antiferromagnetism of Fermion in Optical Lattices with Half-filled p-band

HUI ZHAI, UC Berkeley, KAI WU, Center for Advanced Study, Tsinghua University — We study Fermi gases in a three-dimensional optical lattice with five fermions per site, i.e. the s-band is completely filled and the p-band with three-fold degeneracy is half filled. We show that, for repulsive interaction between fermions, the system will exhibit spin-3/2 antiferromagnetic order at low temperature. This conclusion is obtained in strong interaction regime by strong coupling expansion which yields an isotropic spin-3/2 Heisenberg model, and also in weak interaction regime, by Hatree-Fock mean-field theory and analysis of Fermi surface nesting. We show that the critical temperature for this antiferromagnetism of a p-band Mott insulator is about two orders of magnitudes higher than that of an s-band Mott insulator, which is close to the lowest temperature attainable nowadays.

4:42PM S14.00012 Stripe Formation and Superfluidity Correlation on Two-dimensional Optical Lattice: DMRG Studies for n-leg repulsive Hubbard model

MASAKI MACHIDA, MASAHIKO OKUMURA, SUSUMU YAMADA, CCSE, Japan Atomic Energy Agency — In order to predict strongly-correlated behaviors on two-dimensional (2-D) optical lattice, we employ the parallel density matrix renormalization group (p-DMRG) method and examine 2-D repulsive (square-lattice) Hubbard model. In the presentation, we firstly suggest that box shape trap enables to observe intrinsic properties of the Hubbard model in a fixed doping in contrast to the harmonic trap bringing about wide spatial variations of atom density profiles. Next, we show atomic density profile on 4-leg repulsive Hubbard model with the open boundary condition under the box trap. The variation parameters in the simulation are the doping rate below the half-filling and the repulsive interaction \( U/t \). As a result, we find that stripe formations are universal in a low hole doping regime and the stripe sensitively changes its structure with variations of \( U/t \) and the doping rate. A striking feature is that a stripe by a hole pair turns to one by a bi-hole pair when entering a limited strong \( U/t \) range. Furthermore, a systematic calculation reveals that the Hubbard model shows a change from the stripe to the Friedel oscillation with increasing the doping rate.

4:54PM S14.00013 Superfluidity of fermions with repulsive on-site interaction in an anisotropic optical lattice near a Feshbach resonance

BIN WANG, LUMING DUAN, University of Michigan, Ann Arbor — We present numerical analysis of ground state properties of the one-dimensional general Hubbard model (GHM) with particle assisted tunnelling rates and repulsive on-site interaction (positive-U), which describes fermionic atoms in an anisotropic optical lattice near a wide Feshbach resonance. Our calculation uses the time evolving block decimation algorithm, which is an extension of the density matrix renormalization group and provides a well controlled method for one-dimensional systems. We show that the positive-U GHM, when hole doped from half-filling, shows up a phase with coexistence of quasi-long-range superfluid and charge-density-wave orders. This feature is different from the property of the conventional Hubbard model with positive-U, indicating the particle assisted tunneling in the GHM could bring in qualitatively new physics.

5:06PM S14.00014 Predicted itinerant ferromagnetism with cold fermions in optical lattices

SHIZHONG ZHANG, Department of Physics, University of Illinois at Urbana-Champaign, CONGJUN WU, Department of Physics, University of California, San Diego — Itinerant ferromagnetism is one of the central topics in condensed matter physics. Ferromagnetism is intrinsically strong coupling physics which does not have a weak coupling limit, i.e., spontaneous spin polarization requires strong interactions to overcome the kinetic energy cost. In spite of its importance, ferromagnetism has not received enough attention in the cold atom community because the system is unstable to molecular formation if the interaction is tuned close to resonance from the positive side of the Feshbach Resonance. To overcome this difficulty, we instead propose to realize the ferromagnetic state in the p-orbital honeycomb lattice by taking advantage of its flat band structure. Due to the divergent density of states, even weak repulsions can drive the ferromagnetic transition while ensure the stability of the system. This will open up a new opportunity to investigate ferromagnetism with precise controllability and to realize spin transport and even spintronics applications with cold atoms.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S15 GQI: Superconducting Qubits III

Morial Convention Center 207

2:30PM S15.00001 Transmission line cavity as a quantum memory for superconducting phase qubits

K. CICAK, F. ALTMARE, J.I. PARK, M.A. SILLANPAÄ, R.W. SIMMONDS, National Institute of Standards and Technology, Boulder, CO 80305 USA — A superconducting transmission line cavity coupling two phase qubits has already proven useful as a bus for coherent state transfer\(^1\). In this talk we will discuss our efforts in extending the work of Sillanpäät al\(^2\) to use a transmission line as a short term memory element.

\(^1\)Current Address: Helsinki University of Technology, Low Temperature Laboratory, Finland

\(^2\)NATURE 449, 438-442 (2007)
2:42PM S15.00002 Coplanar resonators as computational elements in a superconducting qubit architecture, MAX HOFHEINZ, E.M. WEIG, R.C. BIALczAK, H. WANG, N. KATZ, M. NEELEY, E. LUCERO, A.D. O’CONNELL, M. ANSMANN, J. WENNER, D. SANK, I. STORCH, J.M. MARTINIS, A.N. CLELAND, UC Santa Barbara — We are coupling a superconducting phase qubit, implemented using a current-biased Josephson junction, to a high-Q coplanar waveguide resonator. The interaction between the qubit phase and the resonator can be controlled by tuning the qubit frequency into and out of resonance with the resonator, a tuning that can be achieved dynamically over times short compared to the Rabi time. By combining the quantum control flexibility of the phase qubit with the long coherence time and bosonic nature of the resonator, a number of interesting quantum operations can be explored, including long-term phase coherent quantum memory and two-qubit bus architectures. In this talk we will report on our recent progress with this experiment.

2:54PM S15.00003 Entangling phase qubits via a common transmission line cavity, JAE PARK, RAY SIMMONDS, NIST, Boulder — We consider ways of “distributing” entanglement to a number of qubits via a common superconducting transmission line cavity. We propose methods of preparing such states and verifying its preparation.

3:06PM S15.00004 Measuring the quantum states of a superconducting cavity, JAE PARK, FABIO ALTOMARE, KATERINA CICAK, NIST, Boulder, RAY SIMMONDS — We consider the prospects for preparing and measuring some basic quantum states (e.g. number states) of a superconducting transmission line cavity coupled to Josephson-junction qubits.

3:18PM S15.00005 Cooling of a Resonator with Microwave Induced Charge-Phase Qubit Transitions, JANI TUORILA, DAVID GUNNARSSON, ANTTI PAILA, JAYANTA SARKAR, EKRI THUNEBERG, YURIY MAKHLIN, PERTTI HAKONEN, Helsinki University of Technology and University of Oulu — We have studied a circuit QED experiment where a superconducting charge-phase qubit is coupled to an electric r-f-resonator via the phase degree of freedom. The resonator is coupled to a transmission line that allows reflection measurement with narrow band detection. Additionally, the charge degree of freedom is coupled to a mw-signal. The level spacing $\hbar \Delta$ of the qubit is controlled with constant shifts in both degrees of freedom. Multiphoton absorption from both drives can excite the qubit in the case the level separation is equal to the sum of the photon energies. The results of the measurements show asymmetry between the depths of the side-resonances of the basic resonance $\Omega = \omega_\mu$. Also, a non-monotonic AC-Stark shift is observed in the apparent resonance positions. Solutions of the semiclassical Maxwell-Bloch equations of the whole measurement apparatus show that the measured results can be considered as evidence of cooling/heating of the oscillator.

3:30PM S15.00006 Fast tuning of a high Q microwave cavity for qubit cooling, M. SANDBERG, C.M. WILSON, F. PERSSON, G. JOHANSSON, V. SHUMEIKO, T. DUTY, P. DELSING — In 2004 Wallraff et al. [1] demonstrated that an artificial atom in form of a superconducting qubit can exhibit coherent interaction with a superconducting high Q microwave transmissionline resonator. In recent experiments [2,3] similar resonators have been used for coupling and reading out qubits. In these experiments the resonance frequency of the resonator is fixed and the qubit frequency is tuned. Here we present measurements on a superconducting transmission line resonator with a tunable resonance frequency that could be used for qubit cooling [4]. With such a device, qubit gates can be performed while the qubits stay at their optimal points. We demonstrate a tunability of 700 MHz for a 4.8 GHz resonator with a linewidth of 500 kHz and that we can tune the resonance frequency by 330 MHz in a few ns. We show that if the resonator is detuned faster than its decay time the photons inside the resonator will shift their frequency with the resonator.

3:42PM S15.00007 Vacuum Rabi Mode Splitting at High Drive Powers and Elevated Temperatures, J.M. FINK, Department of Physics, ETH Zurich, A. BLAIS, Departement de Physique, Universite de Sherbrooke, R.J. SCHOELKOPF, Departments of Applied Physics and Physics, Yale University, A. WALLRAFF, Department of Physics, ETH Zurich, ETH QUANTUM DEVICE TEAM, YALE CIRCUIT QED TEAM — The circuit QED architecture [1,2] is ideal to probe the nonlinearity of a strongly coupled cavity QED system at high drive powers populating the cavity with a controllable average photon number in the range from $0.1 < n < 100$. While in atomic cavity QED the radiation pressure exerted on the atoms by the drive tends to expel the atoms from the cavity, superconducting qubits remain at a fixed position and maintain constant coupling. This enables us to explore the cross-over from the quantum to the classical regime in the single qubit-field interaction by measuring vacuum Rabi mode splitting spectra. We also investigate the effect of thermal radiation in the cavity leading to a thermal population of excited states in the Jaynes-Cummings ladder, which was theoretically studied in Ref. [3]. Simulations have been carried out in order to determine the optimal set of qubit and resonator parameters needed for first experiments.

3:54PM S15.00008 Observation of Berry’s Phase in a Superconducting Qubit, P.J. LECK, J.M. FINK, Department of Physics, ETH Zurich, A. BLAIS, Departement de Physique, Universite de Sherbrooke, R.J. SCHOELKOPF, Departments of Applied Physics and Physics, Yale University, A. WALLRAFF, Department of Physics, ETH Zurich, ETH QUANTUM DEVICE TEAM, YALE CIRCUIT QED TEAM — In quantum information science, the phase of a wavefunction plays an important role in encoding information. While most experiments in this field rely on dynamic effects to manipulate this information, an alternative approach is to use geometric phase, which has been argued to have potential fault tolerance [1]. Here we demonstrate the controlled accumulation of a geometric phase, Berry’s phase, in a superconducting qubit, manipulating the qubit geometrically using microwave radiation, and observing the accumulated phase in an interference experiment [2]. This is achieved utilizing the excellent phase coherence and qubit control possible in Circuit QED [3]. We find excellent agreement with Berry’s predictions, and also observe a geometry dependent contribution to dephasing.

4:06PM S15.00009 Cooper Pair Box Qubit in the Ultrastrong Coupling Regime, MARKUS BRINK, MICHAEL METCALFE, LUIGI FRUNZIO, VLADIMIR E. MANUCHARYAN, JENS KOCH, TERRI M. YU, STEVEN M. GIRVIN, ROBERT J. SCHOELKOPF, MICHEL H. DEVORET, Yale University — We propose a new superconducting qubit design, where a small Josephson junction is inserted in the central conductor of a coplanar waveguide resonator. In this distributed element design, the resonator provides a negative reactance for the junction, which modifies the charging energy $E_C$ of the junction and places the qubit far in the “Transmon regime”. $E_J \gg E_C$, where $E_J$ is the Josephson energy of the junction. We will discuss design details and show preliminary fabrication and measurement results.
4:18PM S15.00010 Homodyne detection of resonance fluorescence in circuit QED, LEV S. BISHOP, JENS KOCH, Yale University, ERKKI THUNEBERG, University of Oulu, JERRY M. CHOW, STEVEN M. GIRVIN, ROBERT J. SCHOELKOPF, Yale University, YALE CIRCUIT QED TEAM — In circuit QED, the transmon qubit[1] allows long coherence times and strong coupling. In this regime, tuning the qubit into resonance with the cavity leads to vacuum Rabi splitting[2] with two transition peaks very well-resolved in frequency (∼300 linewidths apart). At low probe power, these peaks have Lorentzian shape. As the probe power is increased, each Rabi peak is observed to split into two peaks. Approximating the combined effect for a single mode of the cavity does not account for T1s observed in our system. Here we show a semi-classical approximation for the Purcell effect for a multi-mode cavity which we compare with T1 measurements of several transmon qubits[1]. By designing an appropriate cavity we have improved T1 by a factor of 10.

4:30PM S15.00011 Purcell Effect Limits on the Lifetimes of Transmon Qubits, BLAKE JOHNSON, STEVEN GIRVIN, ROBERT SCHOELKOPF, Yale University, THE YALE CIRCUIT QED TEAM — Here we discuss coherence measurements of the transmon qubit, an optimized Cooper Pair Box geometry. We show experimental verification that sensitivity to 1/f charge noise was exponentially suppressed in the transmon qubit. As a result, the effects of gate charge noise and quasiparticle poisoning have been nearly eliminated, and the qubit was seen to be nearly homogeneously broadened. Following an improvement in relaxation times, dephasing times were measured at over a microsecond, nearly twice the relaxation time, without the need of an echo experiment while being tuned over a range of several GHz. The tuning of the qubit excitation energy shows strong agreement with a quantum mechanical calculation of the Purcell effect for a single mode of the cavity.

4:42PM S15.00012 Suppressing Charge Noise Decoherence in a Transmon Qubit, JOSEPH SCHREIER, STEVEN GIRVIN, ROBERT SCHOELKOPF, Yale University, YALE CIRCUIT QED TEAM — We show that charge noise is exponentially suppressed by employing a multi-mode cavity which we compare with T1 measurements of several transmon qubits[1]. By designing an appropriate cavity we have improved T1 by a factor of 10.

4:54PM S15.00013 Circuit QED with phase-biased qubits, JEROME BOURASSA, ALEXANDRE BLAIS, Universite de Sherbrooke, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University, YALE CIRCUIT QED TEAM — Coupling of a superconducting charge qubit to a transmission line resonator has been shown to lead to the very strong coupling regime of cavity qubit[1]. In this talk, we will discuss an alternative approach to circuit QED based on the cavity bifurcation amplifier[2] and where a qubit is directly embedded in the resonator’s center line. We will show that this type of phase bias leads to very strong coupling and/or non-linearities. Readout, decoherence rates and coupling of qubits in this architecture will be discussed. [1] A. Wallraff et al., Nature 431, 162 (2004). [2] M. Metcalf et al., PRB 76, 174516 (2007).

5:06PM S15.00014 Quantum walk on a circle in phase space via superconducting circuit quantum electrodynamics, BARRY SANDERS, PENG XUE, University of Calgary, ALEXANDRE BLAIS, KEVIN LALUMIERE, University of Sherbrooke — We show how a quantum walk, with a single walker and controllable decoherence, can be implemented for the first time in a quantum quincunx created via superconducting circuit quantum electrodynamics (QED). Two resonators are employed to provide simultaneously fast readout and controllable decoherence over a wide range of parameters. The Hadamard coin flip is achieved by directly driving the cavity, with the result that the walker jumps between circles in phase space but still exhibits quantum walk behavior over 15 steps.

5:18PM S15.00015 Quantum mirror transport of qudits and continuous variables and an implementation in Circuit-QED, JASON TWAMLEY, GERARDO ANDRES PAZ SILVA, STOJAN REBIC, Centre for Quantum Computer Technology, Macquarie University, Sydney — We expand on our previous work [J. Fitzsimons and J. Twamley, Phys. Rev. Lett. 97, 090502 (2006)], to derive a globally controlled automata-like protocol for the perfect transmission of quantum information in a chain made up of qubits or a chain made up of harmonic oscillators. The resulting protocol results in perfect spatial reflection of the entire quantum state of the chain about its midpoint. Quantum information can be encoded and then processed in continuous variables if one can engineer highly squeezed states [S. Lloyd and S. L. Braunstein, Phys. Rev. Lett. 82, 1784 (1999)]. We show that appropriately driving a superconducting coplanar microwave cavity coupled to a Cooper-pair box qubit can generate very high squeezings of the cavity mode. We consider a linear array of coplanar cavities nearest-neighbor coupled by Cooper-pair boxes. By controlling the coupling strengths of the cavities to the coupling-CPB qubits and the decoherence rates of the latter with time, we show that we can initialize the cavities to be in highly squeezed CV states, and then execute globally controlled quantum mirroring of the entire chain of CV qubits. We finally show that with extra control on the end cavities of the chain we can further execute universal CV quantum computation.

Wednesday, March 12, 2008 2:30PM - 5:30PM
Session S16 DBP: Focus Session: General Techniques and Radiation Therapies in Biological Physics
Morial Convention Center 208

2:30PM S16.00001 The Evolution of External Beam Radiation Therapy (EBRT) from a Technological Perspective, NICHOLAS DETORIE, Sibley Memorial Hospital, Washington, DC — Since the discovery of x-rays by Roentgen in 1895 ionizing radiations have been used as a treatment for cancer. Such treatments have been based on either implantation of radioactive materials at the site of disease or by aiming external radiation beams at the diseased site. This later method is referred to as teletherapy because the beams originate from a location outside of the body distant from the disease site itself. A brief review of the basic radiation biology will be given to illustrate the rationale for therapeutic use of ionizing radiation and the effects of beam energy and beam type— particulate or photon. The remainder of the presentation will focus on the technological developments supported by the required physical properties of the beams and their associated characteristics that make them suitable for patient treatments. Chronological highlights will include the following sources or devices: superficial x-rays, orthovoltage x-rays, megavoltage x-rays and Cobalt 60 photons, electron beams, neutron beams, negative pi mesons, protons, and heavy ions. The presentation will illustrate how the physical beam properties have been incorporated into modern radiation treatment devices, many of which are equipped with radiation imaging capability. Such devices include: linacs equipped with multileaf collimators for beam shaping and intensity modulation, the Gamma Knife for precise and accurate irradiation of brain tumors or arterial-venous malformations (AVM), the robotic arm based Cyber Knife, and the Helical Tomotherapy unit.
3:06PM S16.00002 State-of-the-Art External Beam Radiation Therapy: Challenges and Opportunities, JATINDER PALTA, University of Florida — Intensity-modulated radiation therapy (IMRT) and image-guided radiation therapy (IGRT) allow delivery of highly conformal non-convex dose distributions. However, these treatment modalities require precise knowledge of multimodality imaging, internal organ motion, tumor control probabilities, normal tissue complication probabilities, three-dimensional dose calculation and optimization, dynamic beam delivery of non-uniform beam intensities, and most importantly the knowledge of uncertainties in the radiation therapy planning and delivery process. These uncertainties arise from a variety of sources throughout the whole process that consists of three distinct steps: imaging, planning, and delivery. In the imaging step, 3D patient information is obtained for treatment planning. Any problem in the acquisition, transfer, conversion, registration, or use of imaging data can lead to increased geometrical uncertainties. Dose calculation algorithms have inherent errors, because they are based on approximate solutions to a complex physical situation. The assumptions of a RTP system in modeling a treatment machine significantly impact dose calculation accuracy. The accuracy of the beam geometry depends on the tolerance of each machine parameter and the magnitude of setup errors. Therefore, one must clearly identify and account for all sources of error in imaging, treatment planning, and delivery process to understand the uncertainty in dose delivered to a patient with IMRT/IGRT. It is necessary to properly account for these uncertainties in radiation therapy to improve the accuracy of the dose delivered to patients. This presentation will provide the framework and guidance to safely implement these technologies in the clinic.

3:42PM S16.00003 Technological Advances in Proton Therapy, JAMES MCDONOUGH, University of Pennsylvania — Proton therapy has interested radiation oncologists since the 1946 paper by Robert R. Wilson describing the energy deposition of proton beams and suggesting it would be more suitable for radiation treatments than beams of x-rays. For all its proposed benefits, only 25,000 or so cancer patients worldwide have been treated with high-energy proton beams over the last fifty years. However, during the past decade that number has started to rapidly increase. In the United States alone the number of dedicated facilities has grown from two to five in the last three years and will likely double again by the end of the current decade. We will soon be treating as many patients in one year as was treated during the first fifty years of proton therapy. Surprisingly, the reason is because of what has been happening in x-ray radiotherapy. Conventional radiotherapy underwent a dramatic change during the past decade with the introduction of multiple advances in imaging technology and beam delivery methods. The imaging advances include both imaging for treatment planning (multislice CT systems, high resolution MRI, and increasing use of PET) and imaging of the target location in the treatment room. The treatment delivery advances, dominated by methods that permit intensity modulated beam delivery, were made possible by increased computational power and more computer control of the treatment delivery. These imaging and beam delivery advances should benefit proton therapy treatments even more than x-ray treatments because of the better conformation of dose to the target that one can achieve with proton beams. However, because of the small size of the proton therapy community it has had difficulty implementing some of the advances made in x-ray therapy. The treatment planning imaging is also used by proton therapy but the on-treatment imaging and the intensity modulation often must be specially developed for each proton therapy system. This talk will present the developments in these areas that are expected to be implemented in the next few years.

4:18PM S16.00004 The active catheter: a novel approach for in-situ dose measurements in brachytherapy, PAUL GUEYE, Hampton University, CENTER FOR ADVANCED MEDICAL INSTRUMENTATION COLLABORATION — Radiation therapy is the primary method for combat cancerous tissues. However, although efficient, it still lacks from having a tool that can enable accurate measurement of the dose delivered to the tissue in-situ. The active catheter concept was taken from a common approach used in nuclear/high energy physics where the target is sometimes constructed so as to provide additional information on the scattering process (i.e., active target). By making the catheters used to transport radioactive sources during brachytherapy treatments becoming sensitive to radiation, one is able to extract dose information in-vivo with minimal to no modification during the treatment process. The technique relies on the use of thin (few 100s microns) scintillating fibers embedded within the brachytherapy device. We will report on two applications of such active catheters pertaining to breast and prostate cancer. The former was applied to the MammoSite® balloon from Cytyc, the accelerated partial breast irradiation technique that is becoming the preferred mode of radiation in breast brachytherapy. Results from water phantom data will be presented and discussed. For the latter, gel phantom tests were performed simulating prostate brachytherapy treatments. Comparison with a treatment planning to these data will be also presented and discussed.

4:30PM S16.00005 The proton and carbon therapy experience of the medical physics group at the Italian Southern Laboratories: Monte Carlo simulation and experiment, G.A. PABLO CIRRONE, C. AGODI, G. CANDIANO, G. CUTTONE, F. DI ROSA, E. MONGELLI, P. LOJACONO, S. MAZZAGLIA, G. RUSSO, F. ROMANO, L.M. VALASTRO, INFN-Laboratori Nazionali del Sud, Catania (I), S. LO NIGRO, Univ. of Catania (I), S. PITTERA, CSFNSM Catania (I), M.G. SABINI, A.O. Cannizzaro, Catania, L. RAFAELE, V. SALAMONE, A.O. Policlinico, Catania (I), C. MORONE, 2nd Univ. of Rome (I), N. RANDAZZO, V. SIPALA, INFN Section of Catania (I), M. BUCCiolini, I. BRUZZI, D. MINICHIELLI, Univ. of Florence — At the Italian Southern Laboratories (LNS) of the Italian National Institute for Nuclear Physics the first, and actually unique, Italian proton therapy center is installed and operating. Up to now, 140 patients have been treated. In this environment a big effort is devoted towards Monte Carlo simulation especially with the GEANT4 Toolkit. The authors of this work belong to the Geant4 collaboration and they use the toolkit in their research programs. They maintain a Monte Carlo application dedicated to the complete simulation of a generic hadron-therapy beam line and take active part in the study of fragmentation processes. Moreover they are working in the development of a prototype of a proton Computed tomographic system. In this work we will report our results in the field of proton and carbon therapy either in the simulation as well as in the experimental side of our activity.

4:42PM S16.00006 Real-time High Resolution Plasmonic nanosensors: pH modulated capta-vidin/biotin binding, JEFFREY ANKER, RICHARD VAN DUYNE, Northwestern University — The ability to observe real-time molecular binding kinetics is important for understanding the functions and interactions of biological molecules. Localized surface plasmon resonance (LSPR) nanosensors exhibit intense extinction and scattering spectra that redshift when molecules bind to their surface. Herein, we use an array of biotin functionalized silver nanoprisms to detect pH-modulated binding and dissociation of captavidin to biotin as a model system. The capta-vidin binds at neutral pH and dissociates at high pH. Spectral shifts are monitored in real-time at high resolution during pH-modulated binding and dissociation cycles over hours. After the first cycle, good reversibility is observed. We also observe pH modulated charging and nanoparticle etching effects which are important experimental parameters and also provide a means to control and modulate the nanoparticle spectra.

1This research was supported by the NSF (Grants EEC-0647560, CHE-0414554, DMR-0520513, and BES-0507036), the National Cancer Institute (1 U54 CA119341-01), and a Ruth L. Kirschstein National Research Service Award (5 F32 GM077020) to J.N.A.
4:54PM S16.00007 Electrical noise gives away presence of cancer or toxins in culture. DAVID RABSON, DOUGLAS LOVELADY, CHUN-MIN LO, University of South Florida — Since 1984, electric cell-substrate impedance sensing (ECIS) has been used to monitor cell behavior in culture and has proven sensitive to morphological changes and cell mobility. Several authors have associated fluctuations in the measured impedance with cellular micromotion; however we are unaware of any previous work applying statistical techniques in order to distinguish two different cell types. We have now demonstrated a method for distinguishing cancerous from non-cancerous cultures of human ovarian surface epithelial cells. Applying similar ideas, we have also determined the presence and concentration of the toxin cytochalasin B in cultures of 3T3 fibroblasts at levels lower than the detection thresholds of other techniques. Measures indicative of both short-time (autocorrelation) and long-time ($1/f^\alpha$ noise in the power spectrum and Hurst and detrended-fluctuation-analysis exponents) show statistically significant differences between the populations. Our measures confirm that the noise from non-cancerous cultures has a higher degree of temporal order, order which we argue must arise from greater coordination of motion between healthy cells than between cancerous ones.


5:06PM S16.00008 Delayed Luminescence and Biophotons from Biological Materials. ERNST KNOESEL, PATRICK HANN, MARIA GARZON, ERIK PFEIFFER, SAMUEL LOFLAND, Rowan University, ROWAN UNIVERSITY TEAM — There has recently been increased interest in the field of biophotonics, since it is a non-invasive technique. Many biological systems, such as yeast, bacteria, leaves, seeds, and algae display the unusual phenomenon of a weak, delayed luminescence on the timescale of seconds to minutes after transient illumination. It is also observed that the time decay of the biophotonic emission is not exponential, even after the delay, and that there can be oscillations in intensity with time, which depend on the duration of the illumination. Results from two types of yeast, i.e. bread yeast, and saccharomyces, as well as those from several types of algae are presented. Possible mechanisms for the source of the ultraweak photon emission are discussed.

5:18PM S16.00009 Dielectric Spectroscopy: noninvasive and fast method for measuring changes in the membrane potential. CORINA BOT, CAMELIA PRODAN, New Jersey Institute of Technology, EMIL PRODAN, Yeshiva University, Stern College for Women — We present a noninvasive and fast method, dielectric spectroscopy, to measure changes in the membrane potential of live cell suspensions, in particular to E. coli. This technique can be applied virtually to any cell suspension, regardless of size or shape and is tested against the traditional one, using voltage sensitive dyes. Precise measurements of the dielectric permittivity $\varepsilon$ and conductivity $\sigma$ of live cells suspensions require prior elimination of the polarization errors. Polarization errors are caused by the ionic content of a buffer, and they affect the total impedance in the low frequency limit. Here, $\varepsilon$ and $\sigma$ represent the fitting parameters; a higher weight is given to each of them for the high frequency domain (3kHz-10kHz), where polarization effects were proven negligible. Measurements were performed in a low electric field (1V/cm) and high frequency domain (3kHz-10kHz), where polarization effects were proven negligible. Measurements were performed in a low electric field (1V/cm) and different buffers are measured, such as HEPES, DMEM with different KCI concentrations. Adding different KCI concentration or ionophores triggers changes in the membrane potential of E. coli. Those changes are measured using dielectric spectroscopy and voltage sensitive dyes.

Wednesday, March 12, 2008 2:30PM - 4:54PM — Session S17 DCMP: Quantum Fluids and Solids II Morial Convention Center 209

2:30PM S17.00001 Phonon-roton modes and a Bose phase in nanoscale liquid $^4$He. JACQUES BOSSY, Institut Neel, CNRS-UJF, Grenoble, JONATHAN PEARCE, National Physical Laboratory, UK, SCHÖBER HELMUT, Institute Laue Langevin, Grenoble, HENRY GLYDE, University of Delaware — We present neutron scattering measurements of the elementary phonon-roton modes of liquid $^4$He confined in nanoporous media. The aim is to compare phonon-roton (P-R) and superfluid density measurements in helium at nanoscales and in disorder. A specific goal is to determine the region of temperature and pressure in which well defined phonon-roton modes (and therefore BEC) exist and compare this with the superfluid region. In 25 $\AA$ mean pore diameter gel similar Yamamoto et al.[1] find that the superfluid phase extends up to a temperature $T_s \approx 1.4$ K at saturated vapor pressure (SVP) (p = 0) and up to a pressure $p_s \approx 34$ bar (T ~ 0). There is apparently a Quantum Phase Transition at $p_s \approx 34$ bar[1]. We find well defined P-R modes (BEC) extend above $T_s$ at SVP (up to $T_s \approx 2.17$ K) and to pressures above $p_s$ (up to a pressure $p \approx 36.3-36.8$ bars at T ~ 0 but no modes above this pressure). This suggests that there is a Bose glass phase consisting of local regions of BEC (fragmented BEC) separated by regions with no BEC surrounding the superfluid phase at all p and T. We compare this phase diagram with other dirty Bose systems. [1] Yamamoto et al. Phys. Rev. Lett. 93, 075302 (2004).

2:42PM S17.00002 Elastic transmission of atoms through superfluid $^4$He, YAROSLAV LUTSYSHYN, J. WOODS HALLEY, University of Minnesota — We investigate completely elastic transmission of atoms through a slab of strongly interacting helium superfluid by diffusion Monte Carlo (DMC) method. Both quasiparticle and condensate mediated modes of transmission have been predicted[1,2] but only quasiparticle mode has been observed[3,4]. We performed numerical calculations of the transmission probability using DMC with a modified fixed-node approach to find the phase shifts of scattering states for elastic transmission process of atoms incident normal to the surface of a free standing helium slab. Transmission coefficients for different energies of the incident atom were computed. Preliminary results for the group velocity of a transmitted wave packet hint at rapid transmission with times characteristic of the virtual condensate mediated process. This work was supported in part by the University of Minnesota Supercomputing Institute.


2:54PM S17.00003 Experimental Observation of Quantized Vortex Reconnection and Turbulence in Superfluid Helium$^1$, MATTHEW PAOLETTI, University of Maryland, KATEPALLI SREENIVASAN, International Centre for Theoretical Physics and University of Maryland, DANIEL LATHROP, University of Maryland — We present experimental studies of the first direct visualization of reconnecting quantum vortices and the decay of superfluid turbulence in $^4$He. Micron-sized solid hydrogen particles are used for particle tracking. The cores of the superfluid vortices trap the hydrogen particles, thereby allowing direct visualization of the dynamics of the line-like defects. We generate superfluid turbulence by driving a thermal counterflow. After pulsing the counterflow, the system relaxes through a cascade of reconnection events. We examine the dynamics of pairs of particles trapped on reconnecting vortices and observe that these particles separate as power-laws in time with a scaling exponent distributed about the predicted value of $1/2$. We show that reconnection leads to power-law tails in the velocity probability distribution function, which is in stark contrast to the Gaussian tails that are ubiquitous in classical turbulence and thermal motion.

$^1$We would like to acknowledge support from NSF, NASA, and the Center for Nanophysics and Advanced Materials at the University of Maryland

3:06PM S17.00004 ABSTRACT WITHDRAWN
3:18PM S17.00005 Scanning Superfluid-Turbulence Cascade by Its Low-Temperature Cutoff, EVGENY KOZIK, Institute for Theoretical Physics, ETH Zurich, and Department of Physics, University of Massachusetts Amherst — Recent advances in experimental techniques have made it possible to explore highly non-trivial short-wavelength physics of low-temperature superfluid turbulence. We analyze the transformation of the (quasi-)classical Kolmogorov cascade into the Kelvin-wave cascade on individual vortex lines at high enough wavenumbers, revealing a chain of three qualitatively distinct intermediate regimes, supported by local-induction motion of the vortex lines, and distinguished by specific reconnection mechanisms. On the basis of this scenario, we develop a theory of low-temperature cascade cutoff, which predicts a peculiar behavior of the quantized vortex line density, $L$, controlled by the frictional coefficient, $\alpha(T) \ll 1$, responsible for the cutoff. Excellent agreement with a recent experiment by Walsme et al. [arXiv:0710.1033]—in which $L(T)$ has been measured down to $T \sim 0.08\,\text{K}$—validates our scenario and allows to quantify the Kelvin-wave cascade spectrum.

3:30PM S17.00006 ABSTRACT WITHDRAWN —

3:42PM S17.00007 Metastable Composite Vortices in Spinor Condensates, ARI TURNER, Harvard University, EUGENIE DEMLER — The ground states of condensates of atoms with spin have a variety of symmetries leading to many types of vortices. The quadratic Zeeman effect produces composite metastable vortices, which are configurations of vortices held together by a force resulting from the Zeeman effect as we explain. If the component vortices were to combine together and react to form a different set of components, then the composite vortex could break up. However, this is prevented by short-range repulsions. Our analysis focuses on the cyclic phase, where the chemistry of the vortices is regulated by the symmetry group of a tetrahedron.

3:54PM S17.00008 Quantum Monte-Carlo study of a two-band boson Hubbard model, SIEGFRIED GUERTLER, The University of Hong Kong, Department of Physics, MATTHIAS TROYER, ETH Zurich, Institute for theoretical Physics, FU-CHUN ZHANG, The University of Hong Kong, Department of Physics — We consider a two band boson Hubbard model, in which the on-site interaction is infinity for the intra-band bosons and repulsive for the inter-band bosons. The on-site inter-band boson interaction may facilitate condensation of vacancies of $a$-boson and interstitials of $b$-boson. We report results of large scale quantum Monte Carlo simulations to study possible supersolid phases of the model.

4:06PM S17.00009 A simple model of thermal conductivity in supersolid Helium, JOSHUA THIBODEAUX, ILYA VEKHTER, Louisiana State University, MATTHIAS GRAF, ALEXANDER BALATSKY, Los Alamos National Laboratories — The recent discovery of the decrease of the torsional oscillator period in solid Helium has led to a renewed interest in a supersolid state. The simplest model for this state is one in which the vacancies undergo Bose-Einstein condensation. Within this model we use the Boltzmann equation to investigate the thermal conductivity of normal $^4\text{He}$ and super solid by considering phonons interacting with a gas of vacancies. We analyze the temperature dependence of the thermal conductivity and specific heat for different vacancy concentrations. We will discuss the consequences of our calculations for existing and future experiments.

4:18PM S17.00010 Local melting at surface and isotope impurities in quantum solids, EMMANUELLE CAPPELLUTI, Research Center SMC, INFN-CNR and Dept. Physics, University La Sapienza, Rome, Italy, GIANLUCA RASTELLI, Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS, Grenoble, France, SERGIO GAUDIO, Dept. Physics, University La Sapienza, Rome, Italy, LUCIANO PIETRONERO, Research Center SMC, INFN-CNR and Dept. Physics, University La Sapienza, Rome, Italy — Surface melting is a well-known phenomenon in classical solids, and it can be related to a local instability of the solid phase close to the surface truncation. In this contribution we employ a self-consistent harmonic approximation to investigate surface melting and local melting close to quantum impurities in quantum solids. We show that surface melting can occur at temperatures much lower than the critical temperature $T_\text{c}$ of the solid phase instability in the bulk. Similar effects are driven by the presence of an isotope substitution. In this latter case, we show that stronger local lattice fluctuations, induced by a lighter isotope atom, can induce local melting of the host bulk phase. Experimental consequences and the possible relevance in solid helium are discussed.

4:30PM S17.00011 A Kosterlitz-Thouless transition in solid $^4\text{He}$?, SERGIO GAUDIO, Dipartimento di Fisica, Universita di Roma, La Sapienza, EMMANUELLE CAPPELLUTI, Dipartimento di Fisica, Universita' di Roma, La Sapienza and ISC, INFN-CNR, Roma Italy, GIANLUCA RASTELLI, Universite' Joseph Fourier, Grenoble, France, LUCIANO PIETRONERO, Dipartimento di Fisica, Universita' di Roma, La Sapienza and SMC Research Center and ISC, INFN-CNR, Roma Italy — We show that the reproducible “Non-Classical Rotational Inertia” signals in solid Helium four are completely ascribable to a Kosterlitz-Thouless transition of liquid $^4\text{He}$ at the grain boundaries. Despite our toy model, we obtain a surprisingly good agreement with the experimental data when comparing the drop of the momentum of inertia. Within our model, we give an estimate of the average size of the grains, which we argue to be limited by the isotopic impurities and show that the signal is inversely proportional to the size of the average size of the grains.

4:42PM S17.00012 Disorder-induced Missing Moment of Inertia in Solid $^4\text{He}$, JIANSHENG WU, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — A microscopic model for the experimentally observed missing moment of inertia in the torsional oscillator experiments on partially-annealed solid $^4\text{He}$ is proposed. We argue that an ordered array of $^4\text{He}$ atoms is a Mott insulator. Disorder destroys the Mott state producing localized states in the gap which beyond a critical value of the disorder induce a superfluid state. Depending on the magnitude of the disorder, we find that the destruction of the Mott state takes place for $d \leq 3$ either through a Bose glass phase (strong disorder and weak disorder) or through a direct transition to a superfluid (intermediate disorder). The critical value of the disorder that separates three region of disorder is shown to be a function of the boson filling, interaction and the momentum cut off. We apply our work to the experimentally observed enhancement $^4\text{He}$ impurities has on the onset temperature for the missing moment of inertia. We find quantitative agreement with experimental trends.

1NSF DMR-0605769

Wednesday, March 12, 2008 2:30PM - 5:42PM –
Session S18 DPOLY: Hybrid Organic-Inorganic Nanomaterials II: Assembly and Fabrication
Morial Convention Center 210
2:30PM S18.00001 Transparent Organic Field-Effect Transistors with Carbon Nanotube Electrodes, ADRIAN SOUTHWARD, VINOD K. SANGUAN, TRACY L. MOORE, ELLEN D. WILLIAMS, MICHAEL S. FUHRER, Dept. of Physics, University of Maryland, College Park, MD 20742-4111 USA, DANIEL HINES, VINCE BALLARATTO, Laboratory of Physical Sciences at the University of Maryland — Carbon nanotube (CNT) films are promising as electrode material for organic field-effect transistors (OFETs). We have fabricated CNT films over large areas by airbrushing and patterned them either using shadow masks, or via photolithography and reactive ion etching. Pentacene thin film transistors bottom-contacted by CNT source/drain electrodes on Si/SiO₂ substrates show moderate mobility (up to 0.1 cm²/Vs) and contact resistance as low as 20 kΩ/cm. The contact resistance varies linearly with the gate voltage, eventually saturating at high negative gate voltage. OFETs were measured at temperatures from 228 to 353.5 K. After accounting for contact resistance, the intrinsic mobility of the transistors is found to be activated in temperature with activation energy between 0.137 and 0.151 eV in reasonable agreement with values in the literature. An all-carbon transparent OFET with CNT source, drain and gate electrodes and polymethylmethacrylate (PMMA) gate dielectric has been assembled on a polyethylene terephthalate substrate by transfer printing, with a field-effect mobility up to 0.06 cm²/(Vs).

1Supported by the Laboratory of Physical Sciences.

2:42PM S18.00002 Directed self assembly of macroscopic nanowires from single-wall carbon nanotubes suspended in aqueous bile-salt solutions, E. K. HOBIE, J. A. FAGAN, M. L. BECKER, S. D. HUDSON, J. CHUN, B. J. BAUER, NIST, M. PASQUALI, Rice — Length purified and chirality enriched single-wall carbon nanotubes (SWNTs) suspended in aqueous bile-salt solutions are found to spontaneously self assemble into macroscopically long straight nanowires, both in confined geometries and on patterned substrates. By patterning surfaces with ordered arrays of hydrophobic and hydrophilic regions, we tailor the self assembly of the nanowires for potential applications in the rapid and cheap fabrication of transparent films with strong directional conductivity. We report a phase diagram, and nanowire self-assembly. The predominant mechanisms for this phase behavior are identified as hydrogen-bonding interactions between contacted bile-salt micelles, which lead to the natural formation of macroporous fibrils, and entropic depletion interactions mediated by free surfactant micelles.

2:54PM S18.00003 Time and Temperature Dependent Rheological Behavior of Single-Walled Carbon Nanotubes Dispersed in Thermoreversible Acrylic Copolymer & Alcohol Solutions, ANDREW B. SCHOC, KENNETH R. SHULL, MSE, Northwestern University, L. CATHERINE BRINSON, MSE & ME, Northwestern University — SWCNT stabilized by A-B diblock and A-B-A triblock copolymers are excellent model systems for studying the relationship between nanotube dispersion and mechanical response. We have investigated the mechanical properties of these materials with low-amplitude oscillatory shear rheological measurements. The solvent used here, 2-ethyl-1-hexanol, is a poor solvent for PMMA (A) at low temperatures but a good solvent for PnBA (B) over the entire temperature range studied. The solubility of the PMMA blocks in 2-ethyl-1-hexanol drives the formation of an elastic gel in the ABA triblock copolymer at low temperatures. In these SWCNT/copolymer materials the storage and loss moduli have been observed to increase with time at fixed temperature. When triblock copolymer gels are used as the matrix, we find that the aging effect is erased by cycling the temperature through the gel transition. An increase in storage modulus is observed upon cooling before the gel formation. However, the moduli revert back to lower values when the gel dissolves on heating. We believe this is a result of semi-permanent nanotube junctions being pulled apart when the gel forms. This reversibility is not observed when the nanowires are dispersed in solutions of diblock copolymer, which do not form gels.

3:06PM S18.00004 Forces between nanorods with end-adsorbed chains in polymer melts, AMALIE FRISCHKNECHT, Sandia National Laboratories — Adsorbed or grafted polymers are often used to provide steric stabilization of colloidal particles. When the particle size approaches the nanoscale, the curvature of the particles becomes relevant. Here I use a classical density functional theory to study the polymer-mediated interactions between two nanorods. The rod are immersed in an athermal, melt polymer blend consisting of: 1) a small fraction of chains of length N=20 with “sticky” ends that are attracted to the rods with energy e/kT so that they form a polymer brush on the rods; and 2) a matrix of chains of length P which have no interactions with the rods. The structure of the brush depends on the nanorod diameter, P, and e/kT. There is an attractive well in the force between the rods near contact, followed by a strong repulsion as the brushes are compressed. The depth of the well increases with increasing P. I will discuss the implications for experimental systems. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

3:18PM S18.00005 Shape and size selection of Au nanorods by reversible flocculation, KYOUNG-WEON PARK, Air Force Research Laboratory, WEI LU, University of Michigan, HILMAR KOERNER, RICHARD VAIA, Air Force Research Laboratory — For gold nanorods (GNRs) synthesized by wet chemical method, spherical particles as a byproduct is inevitable. Efficient and rapid approaches to separate the NRs are critical to optimize the nanostructure-dependent optical properties and not bias conclusions due to existence of spherical impurities. Relatively monodisperse GNRs can be separated from smaller size spheres through repeated centrifugation steps. The number of centrifugation steps, though, must be minimized to avoid irreversible aggregation of rods due to the loss of their capping surfactant. As an alternative, we demonstrate that size selection of GNRs can be achieved by the formation of controlled flocculates of GNRs, driven by an attractive depletion interaction between the NRS induced by surfactant micelles above a critical concentration. The flocculates sediment after a few hours. Separation yields as high as 90 % in number of particles were obtained without any damage to the surface of NRS. Flocculation is reversible upon varying the concentration of surfactant. The effect of the aspect ratio of rods and surfactant micelle structure on the flocculation is discussed with regards to concentration, type and mixing ratio of binary surfactants. The effect of electrostatic interaction is also considered through the impact of different types of electrolytes.

3:30PM S18.00006 Industrial viable process of making nanoparticles of various shapes and interior structures, XIAORONG WANG, Bridgestone Americas, Center for Research and Technology — Over the past 10 years, we attempted to develop industrial viable processes which were of significance in manufacturing the nanoparticles in good quality and large volume. Our effort relied on the self-assembly concepts of block macromolecules in solutions to prepare particles with a hard core made of crosslinked plastics and a soft shell made of low Tg elastomer. Depending on the type and microstructure of the copolymers, the solvent concentration and other process parameters chosen, a variety of shell-core nano-particles of different shapes (spheres, hollow spheres, ellipsoids, cylinders, linear and branched strings, disks and etc.) and sizes (5-100 nm diameter) were reproducibly synthesized. Scale-up studies led to an optimization of the manufacturing process and the production of nanoparticles in large quantities for various product application efforts. The unique performance of those nanoparticles as performance tuning additives and novel rubber reinforcing elements was explored in rubber compounds. This review describes the synthesis methods used to produce the polymer nanoparticles, the technology to modify the particles through functionalization, the means to optimize their performance for specific applications, and the methods to use those particles in rubber compounds. Collaborators: Victor J. Foltz, Kurasch Jessica, Chenchy J. Lin, Jeff Magestrelli, Sandra Warren, Alberto Scuratti, James E. Hall, Jim Krom, Mindaugas Rackaitis, Michael W. Hayes, Pat Sadhu, Georg G. A. Bohm
3:42PM S18.00007 Performance of ZnO nanowire-based hybrid solar cells decorated with CdTe quantum dots deposited by a pulsed electron beam technique\textsuperscript{1}. ROBERTO AGA, RICHARD MU, Fisk University, Nashville TN 37208, KENNETH SINGER, Case Western Reserve University, Cleveland OH 44106 — More efficient nanocomposite hybrid solar cells require facile charge transport to the collecting electrodes as well as photon-to-electron conversion over the broad solar spectrum. In this work, we employ ZnO nanowires (ZnO-NW) as direct conduction pathways for electrons to the collecting electrode by growing them directly on ITO-coated glass substrates. Photovoltaic nanocomposites are then formed by spin-coating of poly(3-hexylthiophene). By decorating the ZnO-NW with CdTe quantum dots deposited by a pulsed electron beam technique, we have extended the photon-to-electron conversion sensitivity beyond 600 nm.

\textsuperscript{1}This research is supported in part by DOD/ARO contracts W911NF-05-1-0453, -05-1-0040, and -04-1-0400, NREL/DOE ACQ-4-33623-03 and NSF-CREST CA:HRD-0420516 and NSF-STC Clips under grant #0423914.

3:54PM S18.00008 Organic and Carbon-based Thin-film Transistors on Flexible Substrates.\textsuperscript{1}. DANIEL R. HINES, A. E. SOUTHARD, J.H. CHEN, M.S. FUHRER, E.D. WILLIAMS, Dept. of Physics, University of Maryland, College Park, MD — Fabrication of organic & carbon-based thin-film transistors (TFT) was achieved on plastic substrates using transfer printing. Each device component (Au electrodes, polymer dielectric layer and semiconductor layer) was printed using only pressure and temperature, eliminating all chemical processing on the device substrate. Pentacene (Pn), poly(3-hexylthiophene) (P3HT), carbon nanotube mats (CNTM) and graphene TFTs were all fabricated on polyethylene terephthalate (PET) substrates, yielding mobilities of 0.237 cm\textsuperscript{2}/Vs for Pn and 0.04 cm\textsuperscript{2}/Vs for P3HT. Bottom-gate CNTM TFTs are p-type, with mobilities of 13.7 cm\textsuperscript{2}/Vs, on/off ratio of 10\textsuperscript{7} and minimal hysteresis. Top-gate graphene TFTs have mobilities of 1.0x10\textsuperscript{3} cm\textsuperscript{2}/Vs for holes and 4x10\textsuperscript{3} cm\textsuperscript{2}/Vs for electrons. P3HT TFTs showed little variation in mobility, but strong variation in threshold voltage for different dielectric layers. These TFTs printed onto plastic substrates with a variety of polymer dielectric layers will be presented and discussed.

\textsuperscript{1}Supported by the Laboratory for Physical Sciences and the UMD-NSF MRSEC.

4:06PM S18.00009 Self-assembled contacts to nanoparticles using metallic Ga droplets. KAN DU, E. GLOGOWSKI, M.T. TUOMINEN, T. EMRICK, T.P. RUSSELL, A.D. DINSMORE, Department of Physics, Department of Polymer Science and Engineering University of Massachusetts Amherst — We demonstrate a pragmatic approach to forming electronic materials and devices, in which metal droplets serve as electrodes and their spacing is controlled spontaneously, via self-assembly, to allow tunneling contact with nanoparticles. We have fashioned devices consisting of droplets of molten metal (Ga). Ga is suspended in acidic solution. Ligand-stabilized Au nanoparticles in solution assembled on the metal surface, as shown by electron microscopy. Coated droplets which are then placed on a substrate and the solvent removed. Electron-transport measurements reveal the Coulomb blockade, in which current is suppressed below a tunable threshold voltage by the energy of charging individual nanoparticles. The threshold voltage for two different sizes of nanoparticles agrees with theory. Our approach provides a straightforward approach to creating nanoscale-precision contacts to nanoparticles and might lead to formation of a large number of microscopic devices from suspension.

4:18PM S18.00010 ATRP of MMA on Asymmetrically Functionalized Gold Nanoparticles. BINGBING WANG, BING LI, CHRISTOPHER LI, Drexel University — Metal nanoparticles have attracted enormous interest due to their unique optical and electronic properties. After the pioneer work of Brust and Schiffrin, a lot of reports have been focused on the modification of the surface of metal nanoparticles with functional groups. However, it still remains a challenging task to synthesize Janus metal nanoparticles, which could potentially lead to directed assembly of the functionalized nanoparticles, an essential step towards using these nanoparticles in real world applications. Asymmetrical gold nanoparticles (AuNPs) modified with two different kinds of polymers on the opposite sides were synthesized using poly(ethylene oxide) single crystals with thiol end groups as the substrate. After the immobilization of AuNPs, room temperature ATRP was performed using the ‘grafting from’ method to obtain asymmetrical AuNPs, which possess the ‘Janus’ nature, i.e. two types of polymer chains were selectively patterned on the different locations of the AuNPs. The asymmetric nature of these AuNPs was demonstrated by NP decoration.

4:30PM S18.00011 DNA guided assembly of well-organized nano-architectures. OLEG GANG, DMYTRO NYKYPANCHUK, MATHEW MÁYÉ, DANIEL VAN DER LÉLIE, Brookhaven National Laboratory — An incorporation of DNA in nano-object design provides a unique opportunity to establish reversible, chemically weak and highly selective interactions between the components of nanosystems. Assembly approaches based on this addressable interactions promise a possibility for creation of rationally designed multicomponent system. However, understanding interplay of interactions, cooperative phenomena leading to phase formation and experimental realizations of ordered phases has remained elusive. Using in-situ x-ray scattering methods, we have studied an assembly kinetics, structure development, and phase formation of DNA-capped nanoparticles on surfaces and in bulk for various DNA assembly schemes. The observed changes in the 2D DNA/nanoparticle array layer reveal an evolution of particle/surface separations and surface coverages. For 3D systems, formation of 3D assemblies with crystalline long-range order in two-component nanoparticle systems was observed. The DNA design, assembly schemes and thermodynamic pathway leading to this crystallization has been explored.

4:42PM S18.00012 Schottky nanodiodes based on electrospun polymer nanofibers: Effect of varying fiber diameter\textsuperscript{1}. RUT RIVERA, NICHOLAS PINTO, University of Puerto Rico - Humacao, ALAN JOHNSON JR., University of Pennsylvania — We report on a simple method to fabricate, under ambient conditions and within seconds, Schottky nanodiodes using electrospun polyaniline nanofibers and an inorganic n-doped semiconductor. The objective of the present work is to investigate the role of surface states on the device operation by fabricating Schottky nanodiodes using fibers of varying diameter. The standard thermionic emission model of a Schottky junction was utilized in analyzing the data. As the fiber diameter gets smaller, the diode rectification ratio and the diode turn-on voltage shifts to lower values, while the diode barrier height and the ideality factor increase. The simple construction and high surface to volume ratio of the nanofiber also makes these devices attractive candidates in the potential fabrication of low power, supersensitive and rapid response reusable sensors.

\textsuperscript{1}This work was supported by NSF.
4:54PM S18.00013 Effects of severe confinement on the structure and dynamics in polymer nanocomposites. S.H. ANASTASIADIS1, K. CHRISPOPOULOU, S. FOTIADOU, Foundation for Research and Technology - Hellas, K. ANDRIKOPoulos, G.A. KOUROUKLIS, Aristotle Univ. of Thessaloniki, Greece, B. FRICK, ILL, Grenoble, France — The structure and dynamics of PEO/Na+ MMT nanocomposites is investigated by XRD, DSC, Raman spectroscopy, and quasi-elastic neutron scattering (QENS). For concentrations up to 20 wt% PEO, the PEO chains within the galleries form either a single- or a double-layer structure of intercalated chains; at higher PEO content only double-layers of intercalated PEO chains are formed within the 0.9nm galleries. For PEO content below 70 wt%, the absence of XRD peaks that can be assigned to crystalline PEO and of any DSC melting transition as well as the observation of broad Raman lines reveal that the PEO chains remain liquid-like. It is only for PEO content higher than 70 wt% that diffraction peaks characteristic of bulk PEO are observed together with sharp Raman lines, proving crystallization of only the excess polymer outside the completely full galleries. QENS investigated the dynamics of PEO in bulk and in confinement. A jump of the bulk PEO dynamics at \( T_m \) is observed whereas the dynamics of confined PEO shows only weak temperature dependence and goes smoothly through the bulk \( T_m \). Sponsered by NATO’s Scientific Affairs Division, by the Greek GSRT and by the EU.

13Also at Aristotle Univ. of Thessaloniki, Thessaloniki, Greece

5:06PM S18.00014 pH and Protein Sensing with Functionalized Semiconducting Oxide Nanobelt FETs. YI CHENG, C.S. YUN, G.F. STROUSE, P. XIONG, Florida State University, R.S. YANG, Z.L. WANG, Georgia Institute of Technology — We report solution pH sensing and selective protein detection with high-performance channel-limited field-effect transistors (FETs) based on single semiconducting oxide (ZnO and SnO2) nanobelts.1 The devices were integrated with PDMS microfluidic channels for analyte delivery and the source/drain contacts were passivated for in-solution sensing. pH sensing experiments were performed on FETs with functionalized and unmodified nanobelts. Functionalization of the nanobelts by APTES was found to greatly improve the pH sensitivity. The change in nanobelt conductance as functions of pH values at different gate voltages and ionic strengths showed high sensitivity and consistency. For the protein detection, we achieved highly selective biotinylation of the nanobelt channel with through APTES linkage. The specific binding of fluorescently-tagged streptavidin to the biotinylated nanobelt was verified by fluorescence microscopy; non-specific binding to the substrate was largely eliminated using PEG-silane passivation. The electrical responses of the biotinylated FETs to the streptavidin binding in PBS buffers of different pH values were systematically measured. The results will be presented and discussed.1 Y. Cheng et al., Appl. Phys. Lett. 89, 093114 (2006). *Supported by NSF NIRT Grant ECS-0210332.

5:18PM S18.00015 On the Miscibility of Polymer / Layered Silicate Nanocomposites. K. CHRISPOPOULOU, I. ALTINTZI, I. ANDRIANAKI, N. KOUFAKI, S. FOTIADOU, S.H. ANASTASIADIS1, Foundation for Research and Technology-Hellas, Greece, E.P. GIANNELIS, Cornell University, Department of Materials Science and Engineering, U.S.A. — In the present work we attempt to control the structure in polymer / layered silicate nanocomposites by understanding and/or altering the interactions between the chains and the surfaces. In this respect, hydrophilic and organophilic systems have been utilized and the final structure of the composites is characterized by X-Ray Diffraction and Transmission Electron Microscopy. The effect of the solvent quality on the final structure, in the case of solution mixing, has been examined and the results are compared with the respective obtained from melt intercalation whereas the role of the chemical structure or of the different glass transition temperature of the polymer has been evaluated. In the case of very immiscible systems like for example polyolefin/silicate composites the effect of a more polar additive has been examined. Phase separated up to exfoliated structures can be obtained in a controlled way by varying the compatibilizer to organoclay ratio. Sponsored by NATO’s Scientific Affairs Division, by the Greek GSRT and by the EU.

13Also at Aristotle Univ. of Thessaloniki, Thessaloniki, Greece

5:30PM S18.00016 Magnetic fluorescent particles with polypeptide shell. SREELATHA S. BALAMURUGAN, PAUL S. RUSSO, Department of Chemistry, Louisiana State University, Baton Rouge, DR. PAUL S.RUSSO TEAM — Magnetic fluorescent particles with a hydrophobic polypeptide shell were synthesized and characterized. The first step was the preparation of an iron oxide magnetic core from ferric chloride and ammonia, and ethanol were added. A mixture of tetraethoxy silane, a complex of fluorescein isothiocyanate (FITC) with 3-aminopropyl triethoxy silane (APTES), ammonia, and ethanol were added.

Also at Aristotle Univ. of Thessaloniki, Thessaloniki, Greece

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S19 DMP: Focus Session: Dopants and Defects in Semiconductors III
Morial Convention Center 211

2:30PM S19.00001 Stoichiometry driven impurity configurations in compound semiconductors. A.K. RAMDAS, Purdue University — As is well known, crystal growth of defect-free compound semiconductors, in contrast to elemental, is inherently limited by non-stoichiometry. High resolution infrared spectroscopy of localized vibrational modes can display unique signatures which reveal the structure of stoichiometry related defect-impurity complexes. The talk will focus on II-VI semiconductors in which group II cations are replaced with a group IIA or a 3d-transition metal. The effect of the solvent quality on the final structure, in the case of solution mixing, has been examined and the results are compared with the respective obtained from melt intercalation whereas the role of the chemical structure or of the different glass transition temperature of the polymer has been evaluated. In the case of very immiscible systems like for example polyolefin/silicate composites the effect of a more polar additive has been examined. Phase separated up to exfoliated structures can be obtained in a controlled way by varying the compatibilizer to organoclay ratio. Sponsored by NATO’s Scientific Affairs Division, by the Greek GSRT and by the EU.

13The investigation was carried out with support from the National Science Foundation (DMR 0405082 and 0705793) in collaboration with G. Chen, I. Miotkowski, J. Bhosale, and S. Rodriguez.

3:06PM S19.00020 ABSTRACT WITHDRAWN —
3:18PM S19.00003 Carrier compensation in semi-insulating CdTe1, MAO-HUA DU, DAVID SINGH, Materials Science & Technology Division and Center for Radiation Detection Materials and Systems, Oak Ridge National Laboratory — Carrier compensation in semi-insulating CdTe has been attributed to the compensation of surplus shallow acceptors by deep donors, usually assumed to be Te antisites. However, our first-principles calculations show that intrinsic defects should not have a significant effect on the carrier compensation due either to lack of deep levels near midgap or to low defect concentration. We demonstrate that an extrinsic defect, $O_{T\ell}$-$H$ complex, may play an important role in the carrier compensation in CdTe because of its deep electronic character and reasonably high concentration. Our findings have important consequences for improving device performance in CdTe-based radiation detectors.

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

3:30PM S19.00004 Gadolinium Doping in ZnTe1, Z.X. MA, Lawrence Berkeley National Lab., LEI LIU, LBNL, UC Berkeley, KIN MAN YU, WALADEK WALUKIEWICZ, DALE PERRY, LBNL, PETER YU, LBNL, UC Berkeley, SAM MAO, LBNL, UC Berkeley — We have investigated, experimentally and theoretically, the effects of Gd doping on the structural and optical properties of ZnTe films grown by pulsed laser deposition. A few % of Gd doping was found to reduce the ZnTe lattice constant with no change in the fundamental band gap. When the doping level is increased to >7%, the lattice constant becomes more or less constant, but the band gap increases abruptly by as much as 50 meV. First-principles calculations based on a density-functional theory using the linearized augmented plane wave method were performed using ZnTe supercells containing either isolated defects or defect complexes. The reduced lattice constant on Gd doping can be attributed to the presence of defect complexes involving substitutional Gd ions and neighboring vacancies. The insensitivity of the band gap at lower Gd concentration can be explained by self-compensation of these defects. The increase in the band gap energy at higher concentration is attributed to band-filling effect.

3:42PM S19.00005 First Principles Investigation of H in CdTe, HIROYUKI TAKENAKA, DAVID J. SINGH, MAO-HUA DU, Oak Ridge National Laboratory — CdTe and alloys particularly (Cd,Zn)Te are of interest for radiation detection and other applications. A key issue is obtaining high mobility compensated material with low concentrations of traps. Hydrogen has been shown to play an important role in various semiconductors with both beneficial and deleterious effects. We investigate the effect of H on vacancies in CdTe using supercells. Our results are obtained from the first principles density functional theory calculations using the full potential linearized augmented plane wave method including local orbitals and based on local density approximation. H atoms in Cd vacancies move toward one of Te atoms, which formTd symmetry with Cd in the bulk system. The bond length between H and Te is 1.7 angstrom. This corresponds to a closely spaced Te-H unit similar to OH. We also present H in Te vacancies. We report the electronic structures as well as positron lifetimes. This work was supported by DOE, NA-22.

3:54PM S19.00006 Origin of doping bottleneck in semiconductor quantum dots, SIU-HUIE WEI, National Renewable Energy Lab, JINGBO LI, SHU-SHEN LI, JIAN-BAI XIA, Institute of Semiconductors, Chinese Academy of Sciences — Doping difficulties in semiconductor nanocrystals have been observed and its origin is currently under debate. It is not clear whether this phenomenon is energetic or depends on the growth kinetics. Using first-principles method, we performed systematic study of defects (donors, acceptors, isovalent defects, etc.) in ZnSe quantum dots. We show that the transition energies and defect formation energies of the donor and acceptor defects always increase as the quantum dot sizes decrease. However, for isovalent impurities, the changes of the defect formation energies are rather small. Our study suggests that for donor and acceptor defects, the doping difficulty is mostly due to energetic effects, whereas for isovalent impurities, the doping difficulty is mostly due to kinetic effects. The origin of the calculated trends is explained using simple band-energy-level models.

4:06PM S19.00007 Increased binding energy of impurities near a semiconductor vacuum interface, . PAUL KOENRAAD, INEKE WIJNHEIJMER, JENS GARLEFF, Eindhoven University of Technology, KARIN TEICHMANN, MARTIN WENDEROTH, SEBASTIAN LOTH, R. ULRBRICH, University of Gottingen — We have recently shown that a STM tip can be used as a tool to manipulate the charge state of a single impurity below the cleavage surface of a semiconductor. This manipulation allowed us to determine the binding energy of single donors and acceptors as a function of their depth (up to 1 nm) below the surface. We found that the binding energy strongly increases near the surface. In the case of a Si-donor in GaAs the binding energy increases continuously from 5.6 meV in the bulk to more than 100 meV close to the surface. Our STM techniques also allowed for the determination of the size and shape of the Coulomb field of single ionized donors. We found that the range of the potential is strongly reduced relative to the bulk value. Both the reduced range of the Coulomb potential and the increased binding energy can be related to a reduced dielectric constant and increased effective mass near the surface. We will discuss the implications of these findings.

4:18PM S19.00008 First-principles simulations of GaAs defects: The challenge of Ga pseudopotentials, PETER A. SCHULTZ, O. ANATOLE VON LILIENTHAL, Sandia National Laboratories, Albuquerque, NM — Design of norm-conserving gallium pseudopotentials (PP) has been investigated for density functional theory calculations of defects in GaAs. A converged PP construction is described. We examined the performance in cubic zinc-blende structure phases of GaAs, GaP, and GaN. Computed lattice constants, bulk moduli, and, particularly, band gaps vary greatly depending on PP construction and exchange correlation functional. The Kohn Sham band gaps exhibit a distinctive sensitivity on lattice constant, direct with a strong near-linear dependence at larger lattice constants with crossover to indirect near (within 5%) of the equilibrium lattice constant. Gradient-corrected functionals with a converged PP give a near-zero GaAs gap, a problem for defect calculations. A 3d-core PP “fixes” the band gap, but predicts GaAs defect formation energies different from converged 3d-valence PP. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

4:30PM S19.00009 Computational studies of a 2D tight-binding model of randomly dispersed hydrogenic centers1, JAYSON PAULOSE, Department of Physics, Princeton University, Princeton, NJ 08544; School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, RAVINDRA BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Physics, Princeton University, Princeton, NJ 08544 — The impurity band arising from s-orbitals of randomly dispersed hydrogenic dopants in semiconductors in two dimensions is studied via exact diagonalization of a tight-binding model. Ensemble averaged density of states (DOS) and inverse participation ratio (IPR) of eigenstates are obtained as a function of energy at low to intermediate doping densities, where small clusters of sites are most significant. A similar calculation is done for p-orbitals for comparison. A strong peak in the DOS is seen due to the impurity level. Increasing the density of sites weakens this peak and produces asymmetry in the DOS and the IPR. A nearest-neighbour pair approximation qualitatively explains several features in the DOS at low densities but does not reproduce the singularity. This motivates a comparison to a hierarchically constructed pair model, as well as random bipartite systems, which is pursued further via a renormalization group approach in a concurrent study.

1Supported by NSF Grant DMR-0213706.
4:42PM S19.00010 Quenched singularity in the density of states of 2D random hydrogenic systems1, R.N. BHATT, Department of Electrical Engineering, Princeton University; Princeton Center for Theoretical Physics, Princeton, NJ 08544, ERIK NIelsen, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, JAYSON PAULOSE, Department of Physics, Harvard University, Cambridge, MA 02138 — Delta-doped hydrogenic dopants in semiconductor heterostructures give rise to an impurity band which can be characterized by a two-dimensional tight-binding model with randomly positioned sites. At low densities, the density of states possesses a singularity about the impurity level, which can be understood in terms of the states of a hierarchically constructed set of impurity pairs. As the density is raised, this singularity is quenched due to further neighbors breaking the electron-hole symmetry. The quenching is accompanied by an asymmetry in the density of states, and pair approximations are insufficient to even qualitatively describe the system at higher densities. We motivate and outline a renormalization group technique that captures the quenched singularity and asymmetry in the density of states. This approach motivates the study of random bipartite systems [1], for which it is particularly suited. We compare the results of both types of systems.

1Supported by NSF-MRSEC (DMR-0213706).

4:54PM S19.00011 Negative magnetocapacitance and associated Schottky barrier height changes in lightly doped GaAs , SEFAATTIN TONGAY, ARTHUR HEBARD, University of Florida, Department of Physics, HEBARD LABORATORY TEAM — We investigate the magnetic field response of Schottky barriers formed on GaAs with Si dopant densities of ~3E16 cm⁻³ and ~9E16 cm⁻³. Negative magnetocapacitance of up to 21% at 20K and increasing Schottky barrier height as determined by various impedance measurement techniques are observed. We attribute these effects to a magnetic-field induced increase in the ionization energies of electrons bound to Si impurity atoms, causing shallow impurity electrons to hop to (ionization process) and from (capture process) the conduction band on longer time scales. The effective field at which these effects are seen is a factor of 10⁻³ smaller than it would be in vacuum because of the smaller effective mass and larger dielectric constant of the GaAs host. The dependence of interband hopping on magnetic field decreases the dipole response in the depletion region and gives a corresponding decrease in the measured capacitance. Magnetic field dependent Schottky barrier heights are inferred from linear 1/C² versus bias voltage plots. We note that these magnetic field dependent effects are occurring in the absence of magnetic impurities and thus need to be understood before characterizing the magnetic response of diluted magnetic semiconductors.

5:06PM S19.00012 Thermally activated persistent photoconductivity & donor binding energy in high mobility AlAs QWs , S. dasgupta, c. knaaK, a. Fontcuberta, m. bichler, g. abstreiter, Walter Schottky Institut, TU Munich, Germany, M. Grayson, Walter Schottky Institut and Dept. of Electrical Engineering and Computer Science, Northwestern University, USA — In AlAs, valley index is important quantum number which can help understand interactions. However, important parameters for growth such as donor binding energy and Si doping efficiency were unknown and AlAs quantum wells (QWs) typically did not conduct in dark. We grew series of (001) and (110) oriented double-sided doped n-type AlAs QWs and deduced Si donor binding energy ∆ in Al₀.₄₅Ga₀.₅₅ As and doping efficiency η. They work in dark possibly because dilute charge traps in substrate are screened by backside doping. From dark saturation density for doping series we deduced ∆₈₁₆=65.2 meV [1]. Our studies show thermally activated PPC where sample is illuminated at 4 K and returned to dark without appreciable density increase. As temperature is increased to 30 K, density doubles, indicating shallow binding energy ∆₈₅₁₄=0 meV post-illumination anneal (PIA). Doping efficiency after illumination for (001) facet was found to be η₈₅₁₄=25% and for (110) η₈₅₁₄=17%. With this understanding, we designed (001) AlAs QW with PIA density n=2.4×10¹¹ cm⁻² and mobility μ=4.3×10⁶ cm²/Vs(330 mK), improvement of almost an order of magnitude over published results. [1] Dasgupta, et al. APL (2007)

5:18PM S19.00013 The low-temperature 2D mobility for metallic p-type GaAs Quantum Well , THEODORE CASTNER1, University of Rochester — At T < 1.2K the mobility μ(T) is determined by charged trap ionized impurity scattering (is) and T-dependent screening [1]. μ(T) is calculated with <E(T)> given by an empirical expression T = τₐσ₀/[x + C tanh(η/2)] [x = E/kT, η = T/τ₀ and a 2D DOS that features a pseudogap. μ(T) exhibits a minimum at Tₘₙₐₜ = T/F/2.25 and increases slowly for T > Tₘₜ. The physical reason for this unusual increase in μ(T) is explained. The coefficient C is directly related to μ(T)/μ(Tₘₜ) [4.0 > ratio > 3.6 for p-type GaAs data [2]]. The T-dependent screening η₂(T) = s(T)/s₀ and s(T) is given by μ(T)/μ(Tₘₜ). This s(T) allows the determination of T* [dr/dT = 0] where T* is slightly less than Tₘₜ. The data [2] is an example of ideal 2D behavior. The role of interactions for T < Tₘₜ and T > Tₘₜ will be discussed. [1] F. Stern, PRL 44, 1469 (1980); [2] X.P.A. Gao et al., PRL 93, 256002 (2004).

1emeritus

Wednesday, March 12, 2008 2:30PM - 5:18PM —
Session S20 DMP: Focus Session: Engineering Interfaces for New Materials III: Heterogeneous Interfaces Morial Convention Center 212

2:30PM S20.00001 Epitaxial Growth of Iron and Iron Nitrides on Wurtzite Gallium Nitride (0001)1, WENZHI LIN, JENONGHAM PAK, KANGKANG WANG, ABHIJIT CHINCHORE, DAVID INGRAM, ARTHUR R. SMITH, Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701 — Magnetic transition metal-containing layers on GaN have potential spintronic applications. We explore the epitaxial growth of iron and iron nitride films on wurtzite (0001)GaN(0001). First, we investigate the growth of ∼1.1 nm iron nitride on w-GaN(0001) using rf N₂-plasma molecular beam epitaxy (MBE) and monitor growth with in-situ reflection high energy electron diffraction (RHEED). We find that Fe₃N grows epitaxially with zinc-blende structure and (111)-orientation on w-GaN(0001). To achieve high Fe content, such as Fe₃N₀.₅ and Fe₂N₀.₅, current efforts are aimed at reducing N content in the source gas. In the case of pure Fe deposition, x-ray diffraction and RHEED suggest the epitaxial relationship to be [110]Ga₃N₁₋₀ₓ/[000]GaN with Fe in bcc structure. The assignment is based on lattice spacing measurements as well as angular dependence of the RHEED pattern. In this presentation, most recent results for Fe and Fe₃Nₓ films grown on w-GaN(0001) will be presented.

1This work has been supported by DOE (grant #DE-FG02-06ER46317).

2:42PM S20.00002 Observation of Standing Waves on the GaN(0001) Pseudo (1x1) Surface by Scanning Tunneling Microscopy at Room Temperature , L. LI, Y. QI, G. SUN, M. WEINERT, University of Wisconsin, Milwaukee — The metallic pseudo-1x1 surface, consists of 2 to 2.5 ML Ga on top of the Ga-terminated GaN(0001), provides an ideally confined 2D electron gas (2DEG), which gives rise to complex standing wave patterns. Even at room temperature, these patterns can be observed by scanning tunneling microscopy (STM) and spectroscopy (STS). The analysis of the modulation of the local density of states within various confinement geometries as a function of the bias voltage shows that nearly free-electron like energy dispersive surface states are being probed.
2:54PM S20.00003 Surface Evolution During Sub-Monolayer Manganese Deposition onto Wurtzite Gallium Nitride (000-1) Surface. 

ABHIJIT CHINCHORE, KANGKANG WANG, WENZHI LIN, JEONGIHM PAK, ARTHUR R. SMITH, Nanoscale and Quantum Phenomena Institute - Ohio University — While transition metal (TM)-doped gallium nitride (GaN) films have been explored as potential spintronic materials, the structural and magnetic effects of various TM adatoms on GaN surfaces are not well understood. In this work, we investigate the deposition of sub-monolayer quantities of Mn onto the N-polar GaN(000-1) ×1 surface. First, the GaN surface is prepared by molecular beam epitaxy. The smooth surface is then annealed to remove excess Ga adatoms. Next, the surface is exposed to a dose [approximately 0.05-0.1 monolayer (ML)] of Mn at substrate temperature of 200 °C. Using in-situ reflection high energy electron diffraction (RHEED), we observe the onset of clear 2× periodicity along [1-100] but only 1× along [11-20]. Additional 0.05-0.1 ML Mn doses lead to increasing intensity of the 2/3-order RHEED streaks, while 1/3-order and 1/4-order streaks weaken. For Mn doses up to about 1/3 ML, the surface appears quite smooth, with the RHEED pattern stable upon heating the surface to 600 °C. The results suggest a surface evolution process leading to a well-ordered Mn-containing structure at the GaN(000-1) surface.

3:06PM S20.00004 Van der Pauw and Hall Measurements on Ultra Thin Silicon-on-Insulator.

WEINA PENG, HONGQUAN JIANG, SANGKEUN HA, MADHU THALAKULAM, DONALD SAVAGE, MARK ERIKSSON, MAX LAGALLY, University of Wisconsin Madison — Ultra-thin silicon-on-insulator (UTSOI) provides opportunities to study the role of the surface in electrical transport in Si. Because the Si layers can be as thin as 10 nm, surface states, surface induced band bending, and gap states at the oxide-Si interface dominate the carrier density. Transport measurements provide a sensitive probe of the carriers. Previous measurements of thin Si structures have shown that Si/SiO2 interfaces trap deplete Si of mobile carriers, and sheet resistances reach 1011 ohm/sq for a 20 nm thick sample [1]. Thus, any perturbation to the surface that induces even modest carrier densities can be detected in transport. We perform van der Pauw and Hall measurements on UTSOI structures with a variety of surface modifications, including hydrogen termination and epichlorohydrin surface attachment. UTSOI that was extremely resistive with oxide on both sides undergoes a drop in resistance of more than 3 orders of magnitude after surface modification. Hall and van der Pauw measurements, reveal the density and the sign of the carriers. We discuss the mechanisms for this increased conductivity. [1] Zhang P. et al. Nature 439 703 (2006)


R. RAMPASAD, C. TANG, University of Connecticut — Driven by a need for device miniaturization in the microelectronic industry, Hf-based high-permittivity materials, such as HfO2, have gained interest for their potential application as gate dielectrics. However, undesirable interfacial phases such as Hf silicides and SiOx are known to form and degrade the performance of devices. It has been postulated that these interfacial phases are related to the segregation of O defects (vacancy or interstitial) to the interface. In this work, we examine the thermodynamic and kinetic driving forces for the segregation of isolated and clustered O defects (vacancies and interstitials) to the Si:HfO2 interface. Using first principles density functional theory calculations, we have determined the formation and migration energies per O defect within bulk HfO2 and at the Si:HfO2 interface. Our results indicate that isolated as well as a distribution of point defects display large driving forces for interface segregation, allowing for the formation of silicides and silicates. Thus, while an abrupt Si:HfO2 interface may be stable in the absence of O defects, such an interface is unstable to the formation of other phases in the presence of O defects.

3:30PM S20.00006 Sub-Angstrom Distortions of an Epitaxial Oxide on Silicon (001).

YARON SEGAL, FRED WALKER, J.W. REINER, C.H. AHN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University, ZHAN ZHANG, Argonne National Laboratory — As metal oxide semiconductor field effect transistor (MOSFET) devices are reduced to the nanometer length scale, atomistic control of the silicon-oxide interface is needed in order to fabricate optimally functioning devices. In this work, we present synchrotron x-ray diffraction measurements of a model system, barium oxide grown epitaxially on Si (001), with an interface phase of submonolayer strontium on silicon. Diffraction results show that the 2×1 surface phase that promotes epitaxy transforms into an interface phase between the oxide and silicon, which also has a 2×1 symmetry on the Si (001) surface. Quantitative analysis of the diffraction is consistent with three classes of models; these involve a 2×1 arrangement of alkaline earth metal in the interface phase, sub-angstrom distortions of the oxide film, or a combination of both. These measurements demonstrate how this reconstruction is a true interface phase that can be used to test our current understanding of silicon-oxide interface physics.

3:42PM S20.00007 Experiment and theory on metal/ceramic interfaces.

MANFRED RHLE, Max Planck Institut fr Metallforschung — No abstract available.

4:18PM S20.00008 Theoretical investigation of the interface structure of θ-Al2O3/NiAl(001).

JHY-PIN CHOU, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan — The atomic structure of Ni-Alumina – Al(771) superlattice shows that the compliant oxide causes substantial disorder in the adjacent, soft metal layers. An H “probe atom” is found to bind best in the disrupted metal region, suggesting that this is the locus of initial failure of a protective oxide layer.

4:30PM S20.00009 Calculated atomic arrangement and impurity bonding at a κ-Alumina – Al(771) interface.

PETER J. FEIBELMAN, Sandia National Laboratories — First principles optimization of a κ-Alumina – Al(771) superlattice shows that the incompatible oxide causes substantial disorder in the adjacent, soft metal layers. An H “probe atom” is found to bind best in the disrupted metal region, suggesting that this is the locus of initial failure of a protective oxide layer.

Work supported by the DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering. Sandia is operated by the Lockheed Martin Co. for the U.S. DOE’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
4:42PM S20.00010 Local dielectric constants in metal-oxide and oxide-oxide interfaces: an ab initio approach to address interfacial effects, BORA LEE, CHOONG-KI LEE, SEUNGWU HAN, Ewha Womans Univ., SHANG-HO JEON, BAE-HO PARK, Konkuk Univ. — Recent experiments indicate that the dielectric constants of thin film oxides are strongly affected by interfaces formed between the oxide and metal or between different oxides. Such interfacial effects will be crucial to high-k dielectric stacks employing oxide materials with nanometer thickness. Therefore, systematic studies on interfacial effects are very important for materials selection and process design of gate stacks. In this presentation, we study on local dielectric constants in metal-oxide and oxide-oxide interfaces within the first-principles framework. Firstly, we introduce an efficient method to calculate local dielectric constants by employing slab models exposed to the vacuum. The static as well as optical dielectric constants are obtained from the change in electrostatic potentials upon the application of external electric fields. Our method can be easily adopted using conventional codes without any modification of the program. We apply this method to investigate interfacial dielectric constants in Au/MgO, Ni/ZrO2, Pt/HfO2, Ni/HfO2, Al/HfO2, SiO2/HfO2, and Al2O3/HfO2 interfaces. Our results show the presence of interfacial region with dielectric constants significantly different from that of the bulk. Microscopic explanations will be provided based on the dynamic charges and hardening/softening of phonons.

4:54PM S20.00011 The role of metal/transition metal oxide/organic interface, GUAN-RU LEE, CHIH-I WU, Graduate Institute of Photonics and Optoelectronics, National Taiwan University, Taipei, Taiwan 10617, Republic of China, TUN-WEN PI, National Synchrotron Radiation Research Center, Hsinchu, Taiwan 300, Republic of China — In this paper, we report a study with UPS and XPS data of metal/transition-metal-oxide/organic interfaces. Transition metal oxides are widely used in organic light-emitting (OLEDs) in recently years, such as WO3, ReO3, MoO3, and V2O5. These metal oxides have been proven to be good hole injection layers in OLEDs, interlayers in tandem OLEDs, and nanocomposite electrodes. Although a large number of studies have been made, little is known about the mechanism of metal/transition-metal-oxide/organic interfaces. UPS and XPS data performed by synchrotron radiation research show that these oxides would catch electrons from organic and results in p-type doping in organic material. In addition, there is a significant structure transition from insulating metal oxide to metallic metal oxide. As a result of high work function metallic metal oxides in anode structures and p-type doping organic hole transport layers (HTLs), holes can easily be injected from anode to HTLs. Current-voltage characteristics (I-V) and quantum-efficiency (\(\eta\)) measurements also show the improvement of device performance with insertion of thin transition metal oxides between anodes HTLs.

5:06PM S20.00012 Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111), H. ZHANG, Sichuan University, China, A. SOON, The University of Sydney, Australia, B. DELLEY, Paul-Scherrer-Institut, C. STAMPFL, The University of Sydney, Australia — Iridium-based catalysts are widely used in several important chemical reactions. Despite this, very little is known about the surface structure of the catalyst and the atomic and molecular processes involved. As a first step towards a microscopic understanding, we use density-functional theory, coupled with ab initio atomistic thermodynamics [1], to investigate chemisorption of oxygen on Ir(111), and the stability of surface oxides. We find that for on-surface desorption, oxygen prefers the fcc-hollow site for all coverages considered, where with increasing coverage, the adsorption energy decreases substantially. Subsurface adsorption is found to be highly unfavourable. The most favourable surface-oxide-like structure has a tri-layer-like (OIrO) configuration, which however, the (p, T) phase diagram predicts is only metastable. For practically all conditions, except ultra-high vacuum, the bulk oxide is thermodynamically the most stable, and the only other stable phase predicted is the on-surface (2x2)-O structure for coverage 0.25 ML [2]. These studies point to the possible importance of oxidized iridium for heterogeneous oxidation reactions. [1] C. Stampfl, Catal. Today 105, 17 (2005). [2] H. Zhang, A. Soon, B. Delley and C. Stampfl, submitted to Phys. Rev. B.

Wednesday, March 12, 2008 2:30PM - 5:18PM –
Session S21 DCP: Focus Session: Fundamental Issues in Catalysis III

2:30PM S21.00001 Transient FTIR spectroscopy for probing reaction pathways on Au catalysts1, STEVEN H. OVERBURY, Oak Ridge National Laboratory — Au is now well known to be an active catalyst if the Au particles are sufficiently small, less than about 5 nm. The causes for this structure sensitivity are now beginning to be better understood. Computational modeling and measurements of size dependence on a single catalyst are consistent with activity at sites with low coordination numbers, due in part to flexibility of adsorbate geometry in these sites. Although small size and low coordinate sites are important in catalyzing, e.g. the CO oxidation reaction, there appear to be other factors which control the observed activity as demonstrated by catalyst deactivation and unusual temperature dependence. We have performed studies of CO oxidation over Au/TiO2, Au/SiO2, Au/ZnO/TiO2 and Au/FePO4 catalysts to explore reaction pathways and the causes for activation and deactivation. Three different reactor systems, a fast gas transient FTIR spectrometer, a slower transient DRIFTS cell and a steady state plug flow reactor have been used to correlate activity with surface species. Using this operando approach the elementary steps in the CO oxidation reaction have been explored. Striking differences between the supports are found. The effect of various pre-treatments, the evolution of the surface species during “steady state” reaction and the role of carbonate, oxygen storage, water, hydroxyl upon catalyst activation and deactivation have been explored and will be described. Reaction pathways and mechanisms will be proposed and compared for the different catalysts.

1Research sponsored by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, U.S. Department of Energy.

3:06PM S21.00002 TBD, BRIAN HAYDEN, University of Southampton — No abstract available.

3:42PM S21.00003 Molecular Factors Determining Selectivity in Catalysis1, FRANCISCO ZAERA, University of California — Achieving high selectivities is arguably the main challenge in heterogeneous catalysis for the 21st century. In complex reaction with competing parallel pathways, small changes in the relative values of the different activation energies are sufficient to switch the selectivity of those processes from one product to another. We in our laboratory have been carrying out mechanistic studies on model metal surfaces to try to identify the key factors that control such selectivity. In this talk we will present several examples of increasing subtlety from that work, with focus on the conversion of hydrocarbons. Specifically, we will discuss issues of regioselectivity and stereoselectivity in early dehydrogenation steps, and how those affect selectivity in the conversion of olefins. Time permitting, we will also discuss issues related to the bestowing of enantioselectivity on solid surfaces.

1Research funded by the US National Science Foundation and Department of Energy.
4:18PM S21.00004 The nucleation and growth of ordered Fe and FeO nanoparticles on reconstructed Au(111) surfaces, NEETHA KHAN, CHRISTOPHER MATRANGA, U.S. Dept. of Energy — Iron-based catalysts, including iron oxides, are an important class of materials with relevance to Fischer-Tropsch catalysis and gas-sensing applications. By growing nanostructured particles on single-crystal surfaces, we can create a model system to study size and shape effects on reactivity. We have studied the formation of monolayer thick iron oxide nanoparticles and thin films on the reconstructed Au(111) surface. STM, XPS, ISS, and LEED were used to evaluate the structure and composition of the iron oxide nanoparticles and films as a function of growth conditions. Iron oxide was grown by depositing iron on Au(111), followed by oxidation at room temperature and annealing to 700 K. XPS results indicate that the Fe is oxidized at room temperature, but the STM results indicate that the particles are not ordered until after annealing to 700 K. Atomically-resolved STM images show that at 0.3 ML Fe coverage, iron oxide nanoparticles, pseudo-hexagonal in shape, are formed, with large defects occurring in the corners. STM images of FeO particles over 0.5 ML Fe also show evidence of a non-coincidence overlayer lattice with a short periodicity of 0.25-0.3 nm modulated by a larger periodicity of approximately 3.5 nm. The larger periodicity results from a moiré pattern formed between the iron oxide overlayer and the underlying Au(111) surface.

4:30PM S21.00005 Dynamic structure in Pt nanoclusters on γ-alumina1, F. VILA, J.J. REHR, J. KAS, Dept. of Physics, U. of Washington, R.G. NUZZO, Dept. of Chemistry, U. of Illinois at Urbana-Champaign, A.I. FRENKEL, Yeshiva U. — Pt nanoclusters on γ-alumina exhibit a number of unusual phenomena including large structural disorder and bond-length contraction with increasing temperature. We investigate this behavior for a prototypical 10-atom Pt cluster using real-time, temperature-dependent simulations combining density functional theory/molecular dynamics and x-ray spectroscopy theory. We find that the cluster structure is dynamically varying in shape and topology on a time scale long compared with internal vibrations. Moreover, the clusters are not rigidly attached to the surface and occasionally pick up or discard a PtO bond. This real-time approach suggests that these nanoclusters are comprised of two distinct populations of Pt atoms depending on the charge transfer from the surface, and reproduces many of their unusual properties.

1Supported by DOE Grants DE-FG02-04ER15109 (FV and JJR), DE-FG03-97ER45623 (JJR), DE-FG02-03ER15476 (RGN and AIF), and NIH NCRR BTP Grant No. RR-01209 (JJK), and by DOE computer support at NERSC.

4:42PM S21.00006 In Situ Characterization of Ethylene Hydrogenation on Pt Powder Using Mass Spectrometry-Sum Frequency Generation Technique, BRYAN HSU, Department of Chemistry, Massachusetts Institute of Technology, SHAWN DOUGAL, PAUL STEVENS, MOHSEN YEGANEH, Exxonmobil Research and Engineering Company, Corporate Strategic Research — Bridging the pressure gap has been of paramount importance to the field of surface science. Unfortunately, the available techniques used to characterize catalytic surfaces have all been limited in some degree by a combination of factors (e.g. low pressure regimes, ex situ analysis, and low surface area catalysts), which do not fully replicate industrially relevant conditions. Here, we present in situ observation of ethylene hydrogenation of Pt powder in a high pressure regime. Using total internal reflection sum frequency generation (TIR-SFG) we are able to identify ethyl, ethylidyne, di-sigma-bonded ethylene, and pi-bonded ethylene surface intermediates and find that these are all present under reactive conditions as monitored with mass spectrometry (MS).

4:54PM S21.00007 Dissociation of water and Acetic acid on PbS from first principles1, ALESSANDRA SATTA, PAOLO RUGGERONE, CNR-INFN SLACS, GIOVANNI DE GIUDICI, Dept. Earth Science, University of Cagliari — The adsorption of complex molecules at mineral surfaces are crucial ingredients for understanding the mechanisms that rule the interaction between minerals and the biosphere and for predicting both the stability and the reactivity of minerals. The present work focuses mainly on the early stages of different adsorption reactions occurring at both the cleavage surface and a high-index vicinal surface of galena (PbS). We have studied the dissociation mechanism of water and acetic acid on the galena surfaces by means of ab initio calculations within the framework of density functional theory in the generalized gradient approximation and of pseudopotential approach. The calculated adsorption energies of the molecules indicate the stepped surface as the most reactive, as expected. The free energy surface during the reaction of ab initio calculations within the framework of the density functional theory in the generalized gradient approximation and of pseudopotential approach. The transition metal clusters generated in the gas-phase and deposited on a Au(111) surface. Using a magnetron cluster source, we are able to produce a wide range of heterogenous reactions such as hydrodesulfurization (HDS)2. However, understanding the role of size, structure, composition and support interactions of the MoS2 particles in these heterogenous reactions has not yet been resolved due to the inhomogeneity of commercial catalysts. Work done in our laboratory is geared towards preparing homogenous samples in ultra high vacuum that can serve as model systems for these types of catalytic reactions. We are currently investigating the reactivity of size-selected transition metal clusters generated in the gas-phase and deposited on a Au(111) surface. Using a magnetron cluster source, we are able to produce a wide range of nanocluster stoichiometries including the Mo9S82+ cluster, which has been observed as the metal core of the well-known Chevrel phase2. The work presented focuses on characterization of the Mo9S82+ cluster deposited on a Au(111) single crystal using techniques such as Auger, photoemission spectroscopy, and thermal desorption. In addition, preliminary reactivity studies will be presented of the supported Mo9S82+ cluster with small sulfur containing molecules. 1. Topsoe, H.; et.al; Hydrotreating Catalysis; Springer: New York, 1996. 2. Umarji, A. M.; et.al.; J. Phys. Chem. Solids 1980, 41, 421.

1A.S. and P.R. thank CASPUR and CyberSar for computing support and Fondazione Banco di Sardegna for partial financial support.

5:06PM S21.00008 Characterization and Reactivity of Mo9S8+ on Au (111) via Size-Selected Deposition, MELISSA J. PATTERSON, JAMES M. LIGHTSTONE, StonyBrook University, MICHAEL G. WHITE, Brookhaven National Laboratory/StonyBrook University — Supported MoS2 nanoparticles are known for their ability to catalyze a wide range of heterogenous reactions such as hydrodesulfurization (HDS)1. However, understanding the role of size, structure, composition and support interactions of the MoS2 particles in these heterogenous reactions has not yet been resolved due to the inhomogeneity of commercial catalysts. Work done in our laboratory is geared towards preparing homogenous samples in ultra high vacuum that can serve as model systems for these types of catalytic reactions. We are currently investigating the reactivity of size-selected transition metal clusters generated in the gas-phase and deposited on a Au(111) surface. Using a magnetron cluster source, we are able to produce a wide range of nanocluster stoichiometries including the Mo9S82+ cluster, which has been observed as the metal core of the well-known Chevrel phase2. The work presented focuses on characterization of the Mo9S82+ cluster deposited on a Au(111) single crystal using techniques such as Auger, photoemission spectroscopy, and thermal desorption. In addition, preliminary reactivity studies will be presented of the supported Mo9S82+ cluster with small sulfur containing molecules. 1. Topsoe, H.; et.al; Hydrotreating Catalysis; Springer: New York, 1996. 2. Umarji, A. M.; et.al.; J. Phys. Chem. Solids 1980, 41, 421.

Wednesday, March 12, 2008 2:30PM - 5:30PM
Session S22 DMP DPOLY: Focus Session: Organic Electronics: Contacts and Interfaces
Morial Convention Center 214
2:30PM S22.00001 Energeterics of organic semiconductor interfaces: enhancing injection via chemical doping1. ANTOINE KAHN, Princeton University — Chemical doping of organic molecular films is a powerful way to improve charge injection and transport in organic devices, and to enhance device functionality. The formation of narrow depletion regions at doped organic-conductor interfaces facilitates injection via carrier tunneling through the barrier, and allows the use of moderate work function and non-reactive metals as efficient contacts. P-doping with the electronegative molecule, tetrafluoro-tetracyano-quinodimethane (F4TCNQ), has been used on a number of hole-transport materials. N-type doping is more challenging, often hindered by the energetic requirements of transferring an electron from the dopant HOMO to the host low lying LUMO. We recently demonstrated efficient n-doping of the electron transport material tris2,5-bis(3,5-bis-trifluoromethyl-phenyl)-thieno[3,4-b,h]-n,14,5,8,9,12-hexazatriphenylene (THAP), which has a 4.59 eV electron affinity (EA), with cobaltocene (CoCp, IE = 4.07 eV). We now introduce a stronger n-dopant, i.e. decamethycobaltocene (CoCp*2), and demonstrate n-doping of copper phthalocyanine (CuPc, EA = 3.25 eV). CoCp*2 is found to have a remarkably low IE of 3.30 eV. N-doping is evidenced by a large upward swing of the Fermi-level in the gap of CuPc, and confirmed by current-voltage (I-V) measurements. A 10^3- to 10^5-fold increase in current density of the interface-doped device is compared to the undoped CuPc device is due to enhanced injection. An additional 10^3-fold increase in current density is observed for the uniformly doped device and is attributed to enhanced conductivity of the bulk film. The application of p- and n-doping of CuPc to an organic homojunction p-n diode with a 1.47 eV built-in potential is demonstrated.

3:06PM S22.00002 Electronic Structure of Interfaces and Heterojunction Ambipolar Organic Thin Film Transistor. YONGLI GAO, HUANJUN DING, University of Rochester, HAIBO WANG, DONGHANG YAN, Institute of Applied Chemistry, The Chinese Academy of Sciences — There has been a considerable interest in forming ambipolar organic thin film transistors (OTFTs) due to their advantageous for integrated circuits. Recently, Shi et al. observed a substantial improvement for both the hole and the electron mobility in ambipolar OTFTs based on the heterojunction formed between copper-hexadecafluoro-phthalocyanine (F16CuPc) and 2,5-bis(4-biphenyl) bithiophene (BP2T). We examined the interface formation between F16CuPc and BP2T using ultraviolet photoemission (UPS) and inverse photoemission spectroscopy (IPES). It is observed that in F16CuPc/BP2T the heterojunction is characterized by band bending in both materials, while in BP2T/F16CuPc the band bending is confined in BP2T only. For F16CuPc/BP2T, the band bending of BP2T and F16CuPc are 0.40 and 0.35 eV, respectively. The band bending region is about 15 nm in both materials, from which the Debye lengths of the materials can be deduced. The combination of the band bending and finite Debye lengths may provide an explanation to the observed ambipolar behavior and improved mobility of the OTFTs based on such heterojunctions.

3:18PM S22.00003 Sub-100 nm Contact Effects in Poly 3-hexylthiophene (P3HT) JEFF WORNE, DOUGLAS NATELSON, Rice University — Poly 3-hexylthiophene (P3HT) is a widely studied, versatile material used in organic electronics. Important to understanding the behavior of P3HT lies in its interaction with metal contacts. Contact effects between P3HT and metal electrodes can influence charge injection into P3HT, giving rise to a contact resistance and thereby influencing device performance. The origin of this contact resistance still remains poorly understood, but may result from changes in film morphology near the metal contact, charge transfer and band bending near the contact, or both. Understanding the detailed behavior of the interface between P3HT and metal electrodes will allow for optimization of device behavior. Based on previous work, the voltage drop at the P3HT/silicon interface happens over 100 nm. We have fabricated devices on the tens of nanometer scale that directly probe this region, and present data on the effect of channel length versus device resistance as well as data on the temperature dependence of device resistance for gold and platinum electrodes. Implications for contact engineering will be discussed.

3:30PM S22.00004 ABSTRACT WITHDRAWN

3:42PM S22.00005 Infrared study of charge injection in organic field-effect transistors, ZHIQIANG LI, University of California, San Diego — We present a systematic infrared (IR) spectroscopic study of charge injection in organic field-effect transistors (FET). These experiments have revealed new unexpected aspects of both polymers and molecular crystals. IR spectromicroscopy was employed to image the charges in poly(3-hexylthiophene) (P3HT) FETs. The charge density profile in the conducting channel uncovers a density-dependent mobility in P3HT due to disorder effects. Our IR studies of single crystal rubrene based FETs show that charge transport in these devices at room temperature is governed by light quasiparticles in molecular orbitals. This result is at variance with the common beliefs of polaron formation in molecular solids. The above experiments have demonstrated the unique potential of IR spectroscopy for investigating physical phenomena at the semiconductor-insulator interface in FET devices. This work is in collaboration with G. M. Wang, D. Moses, A. J. Heeger (UCSB), V. Podzorov, M.E. Gershenson (Rutgers), Z. Hao, M. C. Martin (ALS), N. Sai, A. D. Meyerholen, M. F. Calhoun, J. Sanchez, D. Olaya, M. E. Gershenson and V. Podzorov (Rutgers), M. E. Gershenson (Rutgers).

4:18PM S22.00006 Studies of Au/SAMs/PEDOT-PSS/Au tunnel junctions, NAN SUN, MARYA LIEBERMAN, STEVEN RUGGIERO, University of Notre Dame — We report on tunneling through thin organic films. Junctions of the form: Au/SAMs/Polymer/Au were prepared on electronic-grade Si substrates with Self-Assembled Monolayers (SAMs) including octanedithiol (HS-C16H33-COOH). A transitional conducting polymer film PEDOT-PSS was spun on to the SAMs layer, and junctions were completed with a gold film. X-ray photoelectron spectroscopy (XPS) was employed to monitor the quality of the SAMs films. The electron tunneling properties including dI/dV and d2I/dV2 versus bias for the SAMs are discussed.

4:30PM S22.00007 Electronic functionalization of organic semiconductors with self-assembled monolayers VITALY PODZOROV, Rutgers University — Self-assembled monolayers (SAM) are widely used in a variety of emerging applications for surface modification of metals and oxides. Here, we demonstrate a new type of molecular self-assembly: the growth of organosilane SAMs at the surface of organic semiconductors. Remarkably, SAM growth results in a pronounced increase of surface conductivity of organic materials, which can be very large for SAMs with a strong electron withdrawing ability. For example, the conductivity induced by perfluorinated alkyl silanes in organic molecular crystals approaches 10^5 S per square, two orders of magnitude greater than the maximum conductivity typically achieved in organic field-effect transistors (OFETs). The observed large electronic effect opens new opportunities for nanoscale surface functionalization of organic semiconductors with molecular self-assembly. In particular, SAM-induced conductivity exhibits sensitivity to different molecular species present in the environment, which makes this system very attractive for chemical sensing applications [1, 2]. M. F. Calhoun, J. Sanchez, D. Olaya, M. E. Gershenson and V. Podzorov, “Electronic functionalization of the surface of organic semiconductors with self-assembled monolayers”, Nature Materials, Nov. 18, (2007).

4:42PM S22.00008 Impedance Spectroscopy of Organic Thin Film Transistors and Contacts1, DANIEL LENSKI, ADRIAN SOUTHERD, MICHAEL S. FUHRER, Department of Physics and Center for Nanoscience and Applied Materials, University of Maryland, College Park, MD 20742 USA — We have developed a novel method of characterizing organic thin films using a 2- or 3-contact transmission line configuration, in which an AC voltage is applied to the thin film and the phase and magnitude of the current are measured. This simple method can shed light not only on the bulk properties of the semiconductor film, but also on the contacts, by varying the effective length scale probed in the sample. We present the results of transmission line measurements of pentacene thin films, with several types of contacts including thin films of carbon nanotubes.

1This work has been supported by the Laboratory for Physical Sciences.
5:06PM S22.00009 Cross-sectional Imaging of Organic Optoelectronic Devices and Molecularily Assembled Nanostructures1, D.W. STEUERMAN, A. GARCIA, R. YANG, D.S. SEFERSOS, H. WU, D. KORYSTOV, A. MIKAHOLOVSKY, J.P. LOVFANDER, G.C. BAZAN, D.D. AWSCHALOM — As the science of organic optoelectronic devices continuously matures, performance often improves at the expense of molecular and architectural complexity. One widespread approach toward optimization is the use of several polymers and hybrid materials, either as blends or in multiple layers. Tools to provide a thorough understanding of interfacial structure are lacking. Therefore, we employed a dual beam scanning electron microscope/focused-ion beam (SEM/FIB) to create device cross-sections that we subsequently investigated by transmission electron microscopy (TEM). High resolution images of an assortment of devices will be presented, including: interfaces of polymer-electrode, polymer-polymer, polymer-nanoparticles, and oligomer-nanoparticles in fully fabricated devices and optical cavities. We directly observed a variety of polymer-polymer interfaces depending upon solvent casting conditions, annealing treatments, and molecular functionality.

1 We would like to acknowledge support from the NSF and CNID.

5:06PM S22.00010 Trapping carriers in organic field-effect transistors by metal nanoparticles1, YU CHEN, MASAYA NISHIOKA, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota — A thin layer of metallic Au nanoparticles was coated on substrates that were used for organic field-effect transistors, in order to study how the motion of carriers in the organic was affected by metal/organic coupling. A huge reduction of mobility was observed, due to the increase of the characteristic activation energy. We speculate that this follows from the polaronic motion of carriers resulted from the organic/metal coupling, similar to the organic/dielectric coupling. Further experiments demonstrate that the performance of those devices can be adjusted by changing the configurations of nanoparticles.

1 This work was supported by the National Science Foundation through the University of Minnesota Materials Research Science and Engineering Center under Grant NSF/DMR-0212032 and by the U. S. Department of Energy under grant DE-FG02-02ER46004.

5:18PM S22.00011 Charge-retraction time-of-flight technique for mobility measurements in organic materials, JASON WALLACE, University of Rochester, RALPH YOUNG, University of Rochester and Eastman Kodak Company, CHING TANG, University of Rochester, SHAW CHEN, University of Rochester and Laboratory for Laser Energetics — This presentation will explore a recently reported, all-electrical technique, charge-retraction time-of-flight (CR-TOF), for the measurement of charge carrier mobility through an organic layer. Carriers are injected and accumulated at a blocking interface, then retracted. The retraction current transient is nearly indistinguishable from a traditional time-of-flight photocurrent. The CR-TOF technique is validated by measurement of the hole mobility of two well-known compounds using a common hole-blocking layer. An advantage of all-electrical technique is the applicability to sample layers less than 300 nm in thickness. This method also offers new opportunities such as catching charges in the middle of the sample layer and an alternate determination of the transition voltage of organic-organic interfaces.

Wednesday, March 12, 2008 2:30PM - 5:30PM — Session S23 DMP GMAG: Focus Session: Nanostructured Oxides and Thin Films Morial Convention Center 215

2:30PM S23.00001 Synthesis, structure and properties of nanostructured manganites1, ARUP KUMAR RAYCHAUDHURI, S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata -700098, India — Manganites form a fascinating class of multifunctional perovskite oxides with competing interactions that couple the charge, spin and the lattice. The presence of competing interactions (that often have a comparable energy scale) leads to presence of variety of phases in the manganites that can be tuned by substitution (hole concentration), pressure and magnetic field. Interesting classes of phenomena arise when the size is taken to nanoscales where the ground state can be tuned by the size. The size also tunes the nature of the phase transition and the nature of the electronic transport. Interestingly, the primary change in the lattice structures on size reduction that weakens the orthorhombic distortion. The physical properties of the nanostructured manganites are very distinct and different from that seen in related nanostructured transition metal ferromagnetic oxides like the cobaltates. In this talk we will first describe the methods of synthesis of nanostructured manganites in the form of nanocrystals, nanowires and nanostructured films using soft chemical routes. Arrays of the nanostructured manganites can also be made using such techniques as dip-pen lithography using an Atomic Force Microscope. This will be followed by presentation of results on structures using synchrotron X-rays and neutrons that establish the nature of structural changes on size reduction. The structural changes (as established through the above studies) on size reduction tend to enhance the ferromagnetic interaction in the system. Next we will report a number of physical phenomena that arise as a consequence of the size reduction. This will include destabilization of the charge ordered state, change in the nature of the ferromagnetic transition and non-linear conduction that arises in the nanostructured films due to presence of a large number of grain boundaries. At very low temperatures the transport in the manganites become dominated by such effects as intergrain tunneling and Coulomb blockade.

1 Financial support from DST as an Unit is gratefully acknowledged.

3:06PM S23.00002 Epitaxial growth of complex oxide films by a chemical solution method, Q.X. JIA, M. JAIN, H. LUO, E. BAUER, Los Alamos National Lab, H. WANG, Texas A&M University, A.K. BURRELL, T.M. MCCLESKEY, Los Alamos National Lab — In the last several years, complex oxides have become the basis for many revolutionary electronic devices because they exhibit a wide range of electronic properties that conventional metallic elements and covalent semiconductors do not possess. Complex oxide films can be grown by physical vapor deposition, chemical vapor deposition, and chemical solution deposition techniques. One of the challenges in solution-based processes of oxide films has been to produce high quality films and at the same time to control the stoichiometry. Here we describe a new chemical solution method called polymer-assisted deposition (PAD) to grow epitaxial oxide films (such as Ba1-xSrTiO3 and La0.7Sr0.3MnO3). We use a new strategy to control the distribution of metals in solution at a molecular level and a mixture of metal precursor and soluble polymer to form a solution with desired viscosity. By actively binding the metal, the polymer serves to encapsulate the metal to prevent chemical reaction while maintaining a uniform distribution of the metal in solution. This ensures a homogeneous metal distribution and prevents unwanted reactivity that can lead to the formation of undesired phases. The successful growth of epitaxial complex oxide films by PAD suggests that PAD is a feasible alternative approach to the growth of high quality films with desired properties.

3:18PM S23.00003 Tailoring The Magnetic Properties of TiO2 Nanobelts, SHEN V. CHONG, KAZUHIO YAMAKI, KAZUO KADOWAKI, Institute of Materials Science, University of Tsukuba — Over the past decades, titanium dioxide has been discovered to exist in various novel nano-structural forms with high aspect-ratio and good crystallinity. Moreover, the addition of dopants and the self-assembling of foreign molecules on the surface can enrich the physical and chemical properties of this semiconductor, enhancing its versatility and further promoting this metal oxide to be an important nano-based functional material. Herein we report on the doping of TiO2 nanobelts with small amount of cobalt, producing a diluted magnetic semiconductor which display a Curie temperature well above room temperature. Co-doped TiO2 nanobelts were prepared hydrothermally by powdering a piece of CoO, TiO2, and O2 single crystal. The magnetic properties of these nanobelts could be tailored via different heat treatment procedure. Annealing the as-synthesized cobalt titanate in air at 1000 K produced nanobelts which are paramagnetic, while evidence of room temperature ferromagnetism could be observed after the same sample was annealed under vacuum at length. An even more pronounce ferromagnetic behavior was observed when the nanobelts were vacuum annealed direct from the titanate phase. These results again show the importance of oxygen vacancies in unison with the presence of cobalt in inducing room temperature ferromagnetism in this semiconductor.
3:30PM S23.00004 Surface anisotropy and orbital moment in Fe$_3$O$_4$ nanoparticles, X. BATILLE, N. PEREZ, P. GUARDIA, O. IGLESIAS, A. LABARTA, IN2UB-UB. Barcelona, A.G. ROCA, M.P. MORALES, C.J. SERNA, ICMMA-SIC, L.M. GARCIA, F. BARTOLOME, J. BARTOLOME, ICMA-CSIC and U. Zaragoza, J.C. CEZAR, ESRF-Grenoble — Fe$_3$O$_4$ nanoparticles (NP) in the 5-20 nm range were synthesised in the presence of a variety of surfactants (oleic acid, PVA, ...). Saturation magnetization $M_s$ almost reaches the expected bulk value for those surfactants covalently bonded to the NP, being much larger than in those NP with just a protective coating. Thermo-remanence and ac susceptibility demonstrate that the surface anisotropy constant in covalently bonded NP is similar to the bulk value. XMCD confirms the dependence of the magnetic moment on the surface bond and suggests that the orbital contribution is smaller in covalently bonded NP. The occurrence of bulk $M_s$ in Fe$_3$O$_4$ NP may thus be related to the crystal and magnetic state at the surface. This is of relevance in biomedical applications to reduce the strength of the magnetic field required to obtain a high magnetic response, while the issue of the orbital contribution in Fe$_3$O$_4$ is under hot debate. Work funded by Spanish NAN2004-08805-C04-02, NAN2004-08805-C04-01, MAT2006-03999, MAT2005-02454 and CONSOLIDER CSD2006-12, and Catalan 2005SGR0969.

3:42PM S23.00005 Novel Oxide Glass-Based Nanocomposites: Development and Structural Characterization, KRISTINA LIPINSKA-KALITA, Department of Chemistry, University of Nevada Las Vegas, Las Vegas, NV, USA, CARLO SEGREG, Physics Division, UCPS Department, Illinois Institute of Technology, Chicago, IL, USA, PATRICIA KALITA, Department of Physics, University of Nevada Las Vegas, Las Vegas, NV, USA, OLIVER HEMMERS, Department of Chemistry, University of Texas at Austin, Austin, TX, USA, YOSHIMICHI OHKI, Department of Electrical Engineering and Bioscience, Waseda University, Tokyo, Japan, J. CECIL, M. CHAVARIA, Physics Division, UCPS Department, Illinois Institute of Technology, Chicago, IL, USA — Glasses can gain new functionalities when specific crystalline phases of nanometer dimensions are nucleated in them. We have developed a series of optically transparent glass-based composites, containing nanometer-sized crystals dispersed within the isotropic host matrix. The composites were characterized using conventional and synchrotron x-ray diffraction as well as synchrotron x-ray absorption spectroscopy. EXAFS studies of Er-doped, gallium-silica glasses and composites will be presented. As the glasses are treated at elevated temperatures, long-range beta-Ga$_2$O$_3$ is observed to evolve from the initially amorphous local structure. However, the same samples show no significant change in the Er local structure, possibly indicating clustering or preferential of Er in proximity to Ga atoms.

3:54PM S23.00006 A Memristive Switching Model of Two-Terminal Programmable Nanodevices, DMITRI STRUKOV, Hewlett Packard Labs, JULIEN BORGHETTI, DUNCAN STEWART, GREGORY SNIDER, R. STANLEY WILLIAMS, HEWLETT PACKARD LABS PACK — The existence of a fourth passive circuit element was proposed by Chua in 1971 from fundamental symmetry arguments. Although he showed that such a device, which he called a ‘memristor’ (acronym for memory resistor), had many interesting and useful circuit properties, until now no one has presented a physical model or example of such an element. We show here using a simple analytical example that memristance arises naturally in systems for which electronic and atomic transport are coupled under an external bias, and we explore the range of validity of the basic nonlinear circuit model of a more general class of dynamical devices called memristive systems. These results serve as the theoretical foundation for understanding a wide range of hysteretic current-voltage behavior observed in next-generation non-volatile resistive RAM devices, including nanoscale titanium oxide crosspoint switches built in our laboratory.

4:06PM S23.00007 Nano-crystalline structure and catalytic activity of TiO$_2$ supported manganese oxide catalysts, SERGEY MAMEDOV, Horiba Jobin Yvon Inc., PADMANABHA REDDY ETTIREDDY, NEERAJA ETTIREDDY, Chemical and Materials Engineering Department, University of Cincinnati, Cincinnati, OH, USA, PUNIT BOOCHLAND, Department of Electrical and Computer Engineering, University of Cincinnati, Cincinnati, OH, USA — A series of TiO$_2$ supported manganese oxide catalysts were prepared by wet-impregnation method. Raman spectroscopy was used to characterize the structure and chemical environment of these catalysts as well as manganese oxides. Spectra of different Mn-oxides are presented. It was found that there is strong correlation of the position and the width of E$_g$ mode of anatase at 146 cm$^{-1}$ and Mn-oxide(s) concentration. Evolution of Raman spectra described in the frame of the optical confinement model. In this model, the position and width of the Raman band depend on structural disorder and size of nano-crystals. Size of nano-crystal was estimated.

4:18PM S23.00008 Very Low Frequency (<1 mHz) Magnetic Noise in La$_{0.67}$Ca$_{0.33}$MnO$_3$ Films, SUDESHNA SAMANTA, ARUP KUMAR RAYCHAUDHURI, S. N. Bose National Centre for Basic Sciences — We report an occurrence of very low-frequency (<1 mHz) resistance fluctuations (noise) in a rare-earth perovskite manganite film. This fluctuation is distinct from 1/f noise and is larger than that. The fluctuation arises due to coupling to magnetization fluctuation. It reaches a peak close to the ferromagnetic Curie temperature $T_c$. The magnetic nature of the transition has been established by sensitivity of the noise to a very low applied magnetic field (<0.1 Tesla). The magnetization fluctuation has been calculated from the resistance fluctuation using the directly measured magnetoresistance. The magnetization fluctuations show peak at a temperature close to but lower than $T_c$ and shows a nontrivial dependence on the applied magnetic field.

Financial support from Department of Science and Technology, Govt. of India is acknowledged

3:30PM S23.00009 Film Growth and Surface Energy of (100) CrO$_2$, HUNTER SIMS, KRISHNA CHetry, MAIRBEK CHSHIEV, MINT Center and Department of Physics, University of Alabama, ARUNAVA GUPTA, MINT Center and Department of Chemistry, University of Alabama, WILLIAM BUTLER, MINT Center and Department of Physics, University of Alabama — Rutile structure CrO$_2$ can be grown epitaxially on a rutile TiO$_2$ substrate. Surprisingly, growth in the (100) direction is layer by layer even though surface energies evaluated using the VASP code [1] indicate that the surface energy of TiO$_2$ is less than the sum of the surface energy of CrO$_2$ and the CrO$_2$-TiO$_2$ interface energy. It is known however, that CrO$_2$ (100) surfaces spontaneously decompose to form an epitaxial Cr$_2$O$_3$ phase. We have investigated the conjecture that the layer by layer growth of CrO$_2$ results from the formation of a surface layer substoichiometric in oxygen. If the conjectured substoichiometric layer forms, it must be converted to CrO$_2$ on a rutile TiO$_2$ surface. This is of relevance in biomedical applications to reduce the strength of the magnetic field required to obtain a high magnetic response, while the issue of the orbital contribution in Fe$_3$O$_4$ is under hot debate. Work funded by Spanish NAN2004-08805-C04-02, NAN2004-08805-C04-01, MAT2006-03999, MAT2005-02454 and CONSOLIDER CSD2006-12, and Catalan 2005SGR0969.


4:42PM S23.00010 Study of Magneto-Transmission Spectra of La$_{0.7}$Pb$_{0.3}$MnO$_{3-\delta}$ Epitaxial Thin Film$^1$. SIDNEY MALAK, Binghamton University, RYAN CLAYTON-COX, JIRI STEHLIK, JIAN-QING WANG, Binghamton University — Magneto-transmission (MT) of epitaxially grown La$_{0.7}$Pb$_{0.3}$MnO$_{3-\delta}$ was measured. ThermoElectron Nexus 670 FT-IR spectrometer equipped with an electromagnet was used to obtain IR spectra in the range of 350 to 15000 cm$^{-1}$ in various applied magnetic fields up to 1.0 Tesla. For optimal magneto-spectroscopic measurements in transmission, the studied film had a thickness of 190 nm, with a maximum value up to 80% at 320 K in the colossal magnetoconductance (CMR) effect in 5.5 Tesla. It was observed that the MT scale proportionally with the applied magnetic field and was largest at longer wavelengths below 4000 cm$^{-1}$. In this far infrared range, the maximum observed MT value was 4.0 % at 1.0 Tesla. Beyond FIR range the MT curves monotonically decrease with frequency, until the effect vanishes at 12,000 cm$^{-1}$. Such crossover of magneto-spectroscopic responses from IR to optical frequencies is the first evidence of gradual disappearance of the magneto-dynamics at higher frequencies. Compared with the CMR effect, the measured MT property resembled that of the CMR closely in the field range and frequency ranges studied.

$^1$Supported by the National Science Council of the Republic of China

4:54PM S23.00011 Ferromagnetism in Co doped anatase TiO$_2$ thin films mediated by Co-Ti$^{3+}$O$_3$ complexes. MARIA VARELA, Oak Ridge National Lab, KELLI GRIFFIN-ROBERTS, University of Washington, SERGEY RASHKEEV, Idaho National Lab, MATTHEW PANTELIDES, Vanderbilt University, STEPHEN PENNYCOOK, Oak Ridge National Lab, KANNAN KRISHNAN, University of Virginia — The correlation of spherical aberration in the STEM has enabled sub-Angstrom imaging and spectroscopy, and, in favorable cases, direct imaging of light atoms and interstitials. We identify the origin of ferromagnetism in Co$_{0.03}$TiO$_2$ anatase thin films by combining STEM, EELS and DFT calculations. The films are insulating and ferromagnetic at room temperature. Ferromagnetism is enhanced by a post growth vacuum annealing suggesting a defect-mediated mechanism in these films. DFT finds interstitial Co to be energetically preferred over substitutional Co. STEM imaging reveals the interstitials in the predicted sites, and EELS finds reduced Ti in adjacent columns, also predicted by DFT. The combination of STEM-EELS-DFT therefore identifies the defect responsible for the magnetism: an O vacancy binds to the interstitial Co to form a Co-Ti$^{3+}$O$_3$ complex, with a magnetic moment in good agreement with the observed value. Research sponsored by Div. of Materials Sciences and Engineering US DOE, and NSF/ECS 0224138.

5:06PM S23.00012 Nonmetal-metal transition in anatase Nb-doped TiO$_2$. TARO HitsuSUGi, Advanced Institute for Materials Research, Tohoku University, HIDEYUKI KAMISAKA, KOICHI YAMASHITA, HIROYUKI NOGAWA, TETSUKAZU TSURUHAMA, Univ. of Tokyo, SHOICHIRO NAKAO, YUTAKA FURUBAYASHI, NAOMI YAMADA, Kanagawa Academy of Science and Technology (KAST), YUSUHI HIROSE, TOSHIHIRO SHIMADA, TETSUYA HASEGAWA, Univ. of Tokyo — Anatase TiO$_2$ show nonmetal-metal transition on Nb doping. Epitaxial Ti$_{0.94}$Nb$_{0.06}$O$_2$ (TNO) thin film exhibits low electrical resistivity, $\rho \sim 1.7 \times 10^4 \ \Omega$$cm$ at 300 K, comparable to highly-conducting transition metal oxide, ReO$_3$ and Na$_2$WO$_3$. This TNO is an n-type degenerate semiconductor with carrier density exceeding 10$^{21}$ cm$^{-3}$. We have studied the electronic structure of this TNO system using resonant photoemission spectroscopy and compared with first-principles calculations. The first-principles calculations reveal that there is no impurity state arising from Nb doping, and partial density of states of Nb contribute to both valence band and conduction band. These results imply that Nb is highly-hybridized with Ti and O orbitals, resulting in high activation efficiency of Nb which leads to high carrier density in the TNO system. Resonant photoemission spectra clearly show wide band gap without impurity state with Fermi level located in the conduction band.

5:18PM S23.00013 Carrier mediated Ferromagnetism in Cr: In$_2$O$_3$. RAGHAV PANGULURI, P. KHAREL, C. SUKAKAR, R. NAiK, B. NADGORNlj, G. LAwES, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, R. SURYANARAYANAN, LPCES, Cr$_2$O$_3$, ICMnO, Universite Paris-Sud, 91405 Orsay, France, V. M. NAiK, Department of Natural Science, University of Maryland-Dean, Dearborn, MI 48128 — While a number of Dilute Magnetic Semiconducting Oxides (DMSO), when doped with transition metals, exhibit ferromagnetism well above room temperature, most of them are insulating and hence the relationship between the charge carriers and ferromagnetism remains unclear. Here, we investigate a high Curie temperature DMSO, Cr:In$_2$O$_3$, which is made conductive down to low temperatures. Films of various thicknesses ranging from 200 nm to 1100 nm were grown on sapphire substrate by rf sputtering. Upon vacuum annealing, the samples became both magnetic (with the saturation magnetization $\sim 0.07 \mu_B$/Cr) and highly conductive, in contrast to as-prepared samples which were both non-magnetic and insulating. Point Contact Andreev Reflection (PCAR) spectroscopy with the superconducting Sn tip demonstrated significant (50 % ± 5%) transport spin polarization, strongly suggesting that ferromagnetism in Cr:In$_2$O$_3$ is carrier-mediated. We will discuss the implications of these results on our understanding of the nature of ferromagnetic interactions in DMSOs, as well Cr: In$_2$O$_3$ potential applications as a spin injector.

Wednesday, March 12, 2008 2:30PM - 4:54PM — Session S24 DCMP: Fullerenes (not nanotubes) Morial Convention Center 216

2:30PM S24.00001 Magnetic molecules made of nitrogen or boron-doped fullerenes$^1$. CHIH-KAI YANG, Chang Gung University — By using density functional theory we investigate the electronic structure of a fullerene C$_60$ molecule doped with nitrogen atoms. We find that as long as the number of the impurity atoms is odd the doped fullerene turns magnetic, with its magnetic moment determined by the way the impurities are bonded with the carbon cage. For even number of impurities the pairing of the electrons exclude the appearance of magnetism. Similar results can be deduced by Raman and PES measurements which can then be used to assess the density-functional theory results. Although experimental and computed electron-phonon coupling agree on the total magnitude of the coupling, they do not on the contributions of the individual vibrational modes. Density-functional theory calculations indicate that high frequency modes are responsible for most of the coupling whereas experiments suggest that low frequency modes are the dominating contribution. Up to now, only calculations using the local density approximation (LDA) were performed. In this study, we investigate the effect of exact-exchange functionals, such as B3LYP, on the computed electron-phonon coupling of the different vibrational modes.

$^1$Supported by the National Science Council of the Republic of China

2:42PM S24.00002 Electron-phonon coupling in C$_{60}$ using exact-exchange functional. JONATHAN LAFLAMME JANSEN, MICHEL CÔTÉ, Département de physique et Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — The superconductivity in C$_{60}$ doped crystals is now well understood as a phonon mediated interaction. The strength of the electron-phonon coupling can be deduced by Raman and PES measurements which can then be used to assess the density-functional theory results. Although experimental and computed electron-phonon coupling agree on the total magnitude of the coupling, they do not on the contributions of the individual vibrational modes. Density-functional theory calculations indicate that high frequency modes are responsible for most of the coupling whereas experiments suggest that low frequency modes are the dominating contribution. Up to now, only calculations using the local density approximation (LDA) were performed. In this study, we investigate the effect of exact-exchange functionals, such as B3LYP, on the computed electron-phonon coupling of the different vibrational modes.
2:54PM S24.00003 Electron Transfer and Localization in Endohedral Metallofullerenes

SHENYUAN YANG, ICQS and Institute of Physics, Chinese Academy of Sciences; U of Tennessee; ORNL, MINA YOON, ORNL; U of Tennessee, CHRISTIAN HICKE, Michigan State U, ZHENYU ZHANG, ORNL; U of Tennessee, ENGE WANG, ICQS and Institute of Physics, Chinese Academy of Sciences — Endohedral metallofullerenes constitute an appealing class of nanoscale building blocks for fabrication of a wide range of nanomaterials. One open question of fundamental importance is the precise nature of charge redistribution with the carbon cages (C_{60}) upon metal encapsulation. Using ab initio density functional theory, we systematically study the electronic structure of metallofullerenes, focusing on the spatial charge redistribution. For all large metallofullerenes (n > 32), the valence electrons of the metal atoms are all transferred to the fullerene states. Surprisingly, the transferred charge is found to be highly localized inside the cage near the metal cations, rather than uniformly distributed on the surfaces of the carbon cage as traditionally believed. This counterintuitive charge localization picture is attributed to the strong electrostatic-molecular interactions within the systems. These findings may prove to be instrumental in the design of novel fullerene-based functional nanomaterials.

3:06PM S24.00004 Light Alkaline-Earth-Metal Coated Carbon Fullerenes as Effective Hydrogen Storage Media

MINA YOON, ORNL/U; of Tennessee, SHENYUAN YANG, Chinese Academy of Sciences/U. of Tennessee, CHRISTIAN HICKE, Michigan State U, ENGE WANG, Chinese Academy of Sciences, DAVID GEOHEGAN, ORNL; SHENYUAN YANG, ORNL/U. of Tennessee — We propose functionalizing carbon nanostructures with light alkaline-earth metals for use as hydrogen storage media. To support this idea, we investigate the feasibility of coating C_{60} fullerenes with light alkaline-earth metals and analyze the hydrogen storage capacities of the resulting compounds. We find a new and unique binding mechanism responsible for the strong binding between Ca or Sr atoms and C_{60}. Our theory explains experiments showing that C_{60} can be easily covered by a monolayer of Ca or Sr atoms. The coating results in a charge redistribution leading to electric dipolar fields around the metal atoms through which the fullerene becomes a ideal hydrogen-attractor with a binding strength larger than that of alkali carbon complexes but small enough to prevent hydrogen dissociation in the case of transition metal decorated fullerenes. With a hydrogen uptake of more than 8.4wt% and a binding energy of \approx 0.46eV/H2 on C_{60}, Ca is superior to currently used coating elements.

3:18PM S24.00005 An Investigation of Magnetic, Electronic and Structural Properties of Metallofullerenes

S. VINCENT ONG, MEICHUN QIAN, SHIV KHANNA, Dept. of Physics, Virginia Commonwealth Univ., Richmond, VA 23284 — Gadolinium based endohedral metallofullerenes Gd_{x}N@C_{60} functionalized with OH radicals have been found to enhance the relaxivity by orders of magnitude over conventional agents and are being sought as new contrast agents in magnetic resonance imaging (MRI). Using state of the art density functional theory (DFT) in the regime of the local density approximation with the on-site Coulomb interaction (LSDA + U), we have carried out theoretical studies to determine the electronic and magnetic properties of gadolinium-based and lutetium-based nitride fullerenes, namely Lu_{x}Gd_{x}N@C_{60} (x = 1-2). While Gd_{x}N@C_{60} has previously shown promising features as a contrast agent, the idea of replacing gadolinium atoms by lutetium has been proposed to result in a mixed-metal species for multi-modal imaging. Our results indicate that Lu_{2}GdN@C_{60} is the most stable of all possible configurations with a binding energy 16.57 eV, can be considered for use as both an MRI contrast agent, due to gadolinium’s high magnetic moment, and as a potential radioactive therapeutic or diagnostic agent, by neutron activation of a lutetium radioisotope. These results along with details of electronic structure will be presented.

3:30PM S24.00006 First-Principles Investigation of C_{60}-Pd Interface

LAN LI, HAI-PING CHENG — Conductivity and hybridization of C_{60}-Pd nano-system have been investigated using density functional calculations. From analysis of geometry, energetics and electronic structures, the interaction of C_{60} mono-layer and Pd clusters gives rise to electronic charge transfer at the interface and facilitates the dissociation and uptake of hydrogen, which lead to hydrogen storage. The first-principles studies are carried out by self-consistent plane-wave method. The interaction between ions and electrons is described by projector-augmented wave (PAW) approach. In our calculations, the C_{60} monolayer is doped by the Pd_{n} atoms on h-BN with n = 1-4 and 15, but it also forms a metal-C_{60} nano-array with the Pd clusters. Charge transfer occurs at the interface, from the Pd atoms towards the C_{60} monolayer. This electronic property strongly depends on the nature and number of metal atoms. A large amount of charge transfer between the Pd atoms and the C_{60} monolayer indicates a strong interaction under the ionic effect, in contrast with the interaction of the C_{60} monolayer and a metallic surface. The h-BN surface merely gains 0.1 electrons via C_{60}, proving that h-BN is an insulating material. We also find that Pd is a good catalyst for dissociation and storage of hydrogen on the C_{60} molecules. Hydrogen is sufficiently dissociated in the presence of the Pd atoms/clusters, which assists in bonding of the individual H atoms to C_{60}. Dehydrogenation of C_{60}Pd is also discussed in energetics.

3:42PM S24.00007 Investigation of Trapping Positions for Beryllium Atom in C_{60} Fullerene and Electron Densities at 'Be Nucleus

LEE CHOW, ARCHANA DUBEY, H.P. SAHA, UCF Orlando, GARY S. COLLINS, Washington State University, Pullman, R.H. SCHEICHER, Uppsala University, Sweden, N.B. MAHARJAN, Tribhuvan University Nepal, SUNY Albany, S.R. BADU, R.H. PINK, M.B. HUANG, SUNY Albany, T.P. DAS, SUNY Albany, UCF Orlando — We are investigating, using first-principles Hartree-Fock Roothaan procedure, the trapping sites for 'Be atom in C_{60} Fullerene, following broadly the same procedure as in earlier work by our group for trapping of muonium [1]. A number of possible sites, including the center of the C_{60} mono-layer, the position near the fullerene surface both outside and inside C_{60} are being studied including the effect of relaxation in the positions of neighboring C atoms. Electron densities at the 'Be nucleus will be presented for the sites where the binding energy is positive to attempt to understand the observed anomalous electron capture rate compared to other systems where trapped 'Be atom has been studied [2]. Results of our investigations for 'Be atom in graphite and graphene will also be presented for comparison with 'Be in C_{60}. Possible influence of many-body effects will be discussed. [1] O. Donzelli, T. Biere, T.P. Das, Sol. St. Comm. 90 663(1994), Indian J. Phys. 67 (Special Issue) 35 (1993) [2] Ohtsuki et al, Phys. Rev. Lett. 93,112501, (2004)

3:54PM S24.00008 Transfer of a Single Carbon Fullerene at Small Nano-Gap

YOSHIFUMI OSHIMA, YOSHIHIKO KURUI, KUNIO TAKAYANAGI, Tokyo Institute of Technology, PRESTO-JST COLLABORATION, CREST-JST COLLABORATION — A single carbon fullerene shows jump-to-contact behavior in conductance evolution when bringing an electrode close to it. Theoretically, the jump-to-contact behavior has been explained by deformation of the fullerene, but, it has not been proved experimentally. In this study, we investigated the geometry of the fullerene at the moment of jump-to-contact using transmission electron microscope – scanning tunneling microscope system. A single carbon fullerene was synthesized in-situ [1]. We sometimes observed that the single carbon fullerene was transferred back and forth between both electrodes at the bias voltage of 0.6 V when the gap distance became almost 1nm which was still tunneling regime in conductance. Such a transfer was never observed when the bias voltage was lower than 0.1 V. Since the conductance showed the order of 10^{-11} G0 in pulse at the moment of transfer, the fullerene was suggested to be expanded along the gap to have a contact with the opposite electrode. [1] M. Yoshida et al., Jpn. J. Appl. Phys. 46, L67 (2007).
4:06PM S24.00009 Boron Fullerenes: An Electronic Structure Study, ARTA SADRZADEH, OLGA PUPY-SHEVA, Rice University, IHSAN BOUSTANI, Berg Univ Gesamtsch Wuppertal, BORIS YAKOBOSON, Rice University, BORIS I. YAKOBOSON TEAM, IHSAN BOUSTANI COLLABORATION — Using ab initio calculations, we study electronic structure and frequency modes of $C_{60}$, a member of boron fullerenes family made from boron isomorphs of carbon fullerenes with additional atoms in the centers of hexagons. We also investigate geometrical and electronic structural properties of double-rings with various diameters, which are important as building blocks of boron nanotubes, and as the most stable clusters among the studied isomers with more than 36 atoms. Double-rings also appear as building blocks of $C_{60}$. Furthermore, we investigate the possibility of further stabilizing some of fullerenes by depleting them.

4:18PM S24.00010 Magic Number of a Spherical Ca Cluster on $C_{60}$, SUNGJONG WOO, YOUNG-KYUN KOWN, University of Massachusetts Lowell — Since the discovery of fullerenes, there have been a lot of interest in investigating the metal-fullerene clusters. Mass spectrum on the metal(M) covering on a $C_{60}$ complex showed a peak at $M_2C_{60}$. This magic number was theoretically explained using the geometry based on the C-Ca binding. However, such theories could not clearly reveal why the peak at $M_2C_{60}$, especially for calcium clusters, is so prominent compared to smaller number of metal atoms. Using ab initio MD simulations, we have found that for Ca covering with less than 32 atoms, Ca atoms tend to be retracted to a cluster rather than to be bound on each face of $C_{60}$, even though the Ca atoms are deposited symmetrically. Such a cluster does not have specific number of atoms and it is bound to $C_{60}$ through van der Waals interaction. However, once Ca forms a spherical shell with 32 atoms, the structure is quite rigid so that it will not be retracted to a cluster. We have also found that the interaction between an individual Ca atom and each $C_{60}$ face gets loosen so that $C_{60}$ can rotate within a solid phase. The phonon spectrum has been obtained by spectral analysis and electronic orbitals of $Ca_{32}C_{60}$ will also be presented.

4:30PM S24.00011 First principles study of cubane and alkali doped $C_{60}$ solids, YOUNG-MOO BYUN, VINCENT CRESPI, Department of Physics, Penn State University — Alkali doped fullerene ($C_{60}$) solids have been studied widely due to their interesting physical properties. Lately, an experimental group succeeded to dope cubane ($CBH_8$) into the octahedral voids of face-centered-cubic (FCC) $C_{60}$ solids, demonstrating that not only atoms (and polyatomic cations), but also small neutral molecules can intercalate into $C_{60}$ solids. We study the electronic properties of cubane-doped $C_{60}$ solids using first-principles techniques and show that $C_{60}$ solids doped with cubane and alkali metals, in which alkali metals such as K and Rb occupy the tetrahedral voids are energetically favorable. Cubane molecules substantially dilate the $C_{60}$ lattice, resulting in a very large density of states in a single-particle treatment and pronounced tendency towards electronic instability.

4:42PM S24.00012 First principles electronic structure calculation of interstitial P doped $C_{60}$ solid, SHIZHONG YANG, GUANG-LIN ZHAO, DIOLA BAGAYOKO, Physics Department, Southern University and A&M College, Baton Rouge, LA70813 — $C_{60}$ solid has a very low thermo-conductivity that can be utilized to improve the figure-of-merit of thermo-electric devices. The selection of suitable doping elements and doping concentrations in $C_{60}$ bulk semiconductors, for best performance in thermoelectric applications, is of great interest. In this work, we calculated the electronic structure of solid $C_{60}$, interstitially doped with P, at concentrations varying from 1.240 to 1.60. We employed a density functional potential and the plane wave method. Both local density approximation (LDA) and generalized gradient approximation (GGA) potentials were considered. The stability, the electron densities of states, dopant location, carrier type, volume change, and charge transfers of P doped $C_{60}$ were calculated and compared to those of B, N, and Co doped $C_{60}$ solids. In the 1.60 doping case, we found that P doped $C_{60}$ solid is an n-type semiconductor with the dopant energy levels in the band gap, close to the top of conduction band. This work was supported in part by the Department of the Navy, Office of Naval Research (ONR, Grant No. N00014-4-1-0067) and by the National Science Foundation (Award No. HRD050362).

Wednesday, March 12, 2008 2:30PM - 5:42PM – Session S25 DPOLY: Gels and Elastomers Morial Convention Center 217

2:30PM S25.00001 Large strain deformation of hydrophobically modified polyelectrolyte hydrosols, GUILLAUME MIQUELARD-GARNIER, COSTANTINO CRETON, DOMINIQUE HOUDRET, ESPCI — Hydrosols made from charged polyelectrolytes have been widely studied for their ability to absorb large amounts of water. However this occurs usually at the expense of mechanical properties. Because of recent reports describing very tough charged hydrosols, we have investigated the large strain and fracture resistance of novel chemically and physically crosslinked hydrosols. The backbone was polyacrylic acid modified with hydrophobic side groups and subsequently chemically crosslinked with thiol-ene chemistry. We performed compression/decompression experiments up to large strains and found that at polymer concentrations of 5-8 wt% these gels depart significantly from Gaussian behaviour at strains above 150% showing a pronounced strain hardening. We argue that this hardening leading also to a significant increase in ionic strength or the substitution of water with an organic solvent reduces or eliminates the effect implying that it is the charges that cause the hardening and the hysteresis.

2:42PM S25.00002 Creasing instability of surface-attached hydrogels, RYAN C. HAYWARD, VERONICA TRUJILLO, JUNGWOOK KIM, ANESIA BURNS, University of Massachusetts, Amherst — Surface-attached hydrogels provide a convenient means to tune physical properties. Lately, an experimental group succeeded to dope cubane (C8H8) into the octahedral voids of FCC $C_{60}$ solids, demonstrating that not only atoms (and polyatomic cations), but also small neutral molecules can intercalate into $C_{60}$ solids. We study the electronic properties of cubane-doped $C_{60}$ solids using first-principles techniques and show that $C_{60}$ solids doped with cubane and alkali metals, in which alkali metals such as K and Rb occupy the tetrahedral voids are energetically favorable. Cubane molecules substantially dilate the $C_{60}$ lattice, resulting in a very large density of states in a single-particle treatment and pronounced tendency towards electronic instability.

2:54PM S25.00003 Swelling-Induced Deformation of Nanopatterned Polymer Lines, VIJAY TIRU-MALA, CHRISTOPHER STAFFORD, RUI HUANG, LEONIDAS OCOLA, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY TEAM, UNIVERSITY OF TEXAS AT AUSTIN TEAM, ARGONNE NATIONAL LABORATORY TEAM — The deformation behavior of isolated poly(N-isopropylacrylamide) nanolines due to swelling is studied to quantitatively establish the parameters governing their mechanical stability. The features are patterned using electron-beam lithography and are supported on a rigid substrate. In the range of 50-250 nm linewidth, we show that the swollen lines undergo Euler buckling with stable higher order modes due to the constraint for polymer chain expansion at the substrate interface. The critical wavelength for buckling surprisingly increases with decreasing line length. The critical wavelength thus becomes a function of the initial length and decreases dramatically as the line length approaches twice the buckling wavelength for infinitely long lines. A critical length, larger than the buckling wavelength for infinitely long features, exists below which the lines remain mechanically stable regardless of their crosslink density. For sufficiently long lines with height-to-width aspect-ratio in the range 0.5-1.7, the scaling relationship for buckling wavelength vs. linewidth suggests that swelling is anisotropic and is more dominant through height than width. The results established in this study are more generally applicable to nanopatterned polymer lines since buckling instabilities involve simultaneous bending and compression, which deform the material with equal force but in opposite directions.
3:06PM S25.00004 Drop spreading and resorption on gel surfaces1, MEHDI BANAHAD, ADRIAN DAERRD, MSC* Denis-Diderot-University of Paris, LAURENT LIMAT, MSC* CNRS & Denis-Diderot-University of Paris — We have studied the dynamics of liquid drops on agar gels, using a visualisation method which captures the evolution of the free surface. A first remarkable observation is that drops of water deposited on the surface do not spread, although the gel consists of up to 99.7% water and as low as 0.3% agarose. Instead, the drop slowly de-wets and resorbs into the gel which swells locally. If the deposited drop contains surfactants, the dynamics is very different. A sharp circular swelling front develops and progressively invades the whole surface. We study the propagation of this front as a function of surfactant and agarose concentration, and compare its typical properties to similar fronts appearing during mass swelling events of bacterial colonies under the same conditions. The observations reveal the complex nature of gel surface physico-chemistry and its aging, and may be related to recent friction measurements at gel interfaces.

1We acknowledge financial support through an ACI DRAB grant.

3:18PM S25.00005 Anomalous Composition-Dependent Swelling Behavior of Photocrosslinked VP/AA Copolymeric Hydrogels, J. HANNAH LEE, DAVID BUCKNALL, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology — We are investigating the swelling behavior and network structure of vinylpyrrolidone (VP)/acrylic acid (AA) copolymeric hydrogels synthesized using ultraviolet (UV) initiated polymerization. The goal of this work is to develop hydrogels with large expansion volumes but low expansion rates for use in tissue expander applications. In a number of reports, hydrogels composed of VP and AA units have shown that with increasing AA content higher equilibrium swelling ratios (equ) are produced. This behavior is due to higher osmotic pressure induced by the dissociation of carboxyl groups in the AA units into carboxylate anions and hydrogen ions during the swelling. In contrast, in our UV-cured system we found that the value of equ showed a distinct maximum at approximately 50 wt% AA. This anomalous swelling behavior has been studied by measuring the modulus and investigating swelling kinetics as a function of AA content, in addition to the composition and thermal analysis of the dried VP/AA gels. These measurements provide detail of the effective crosslinking density as well as weight between crosslinks for these hydrogels. From these results we propose a model which describes this anomalous behaviour based on the molecular chain structure of the hydrogels.

3:30PM S25.00006 Organogels from Polypeptide-based Block Copolymers, DANIEL SAVIN, DANIEL BERCOCI, SANDEEP NAIK, Department of Chemistry, University of Vermont — A series of AB diblock and ABA triblock copolymers consisting of poly(Lysine) (A) ( = P(Lys(Z)) ) and poly(propylene oxide) (B = PPO) were synthesized and found to form stable, rigid organogels in THF (ca. 1.5 wt.% solutions) at room temperature. In these systems, the protecting group on the P(Lys) side-chains remains intact. As such, the secondary structure of the polypeptide chains retains its helicity over a wide range of solution conditions. Gel formation in these systems results from the assembly of the solvethenphobic P(Lys(Z)) chains, which pack densely in an anti-parallel fashion, minimizing interfacial curvature. These gels exhibited shear-thinning behavior, and as the temperature was heated to 77°C exhibited a gel-sol transition. The gels formed over a time scale of about 10 minutes and had a modulus on the order of 55 Pa. The molecular weight dependence of the gel formation and rheological properties was studied in THF, dioxane and toluene.

3:42PM S25.00007 Soft random solids and their spatial elastic heterogeneity, XIAOMING MAO, PAUL GOLDBART, University of Illinois at Urbana-Champaign, XIANGJUN XING, Syracuse University, ANNETTE ZIPPELIES, University of Goettingen — As a consequence of the disorder that is quenched in at synthesis, random solids are spatially heterogeneous, not only in their structure but also in their response to external conditions. For the case of soft random solids, the heterogeneity in the elasticity is particularly intriguing, owing to its entropic origin and the interplay with incompressibility. We have examined the issue of heterogeneity in the elastic properties of soft random solids by applying replica statistical mechanics to a semi-microscopic model of a random network medium [1]. We have characterized the elastic heterogeneity by random residual stress and Lame coefficient fields, and have determined the statistics of these quantities. We have found that correlations involving the residual stress field are long ranged, and are governed by a universal parameter that also determines the mean shear modulus. Non-affine elastic deformations in soft random solids can also be also studied within this framework. [1] X. Mao, P. M. Goldbart, X. Xing and A. Zippelius, Europhys. Lett. 80, 26004 (2007).

3:54PM S25.00008 Effective removal of entanglement points by network dilution, JOSHUA D. MCGRAW, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — A polymer system in which the chains are much longer than the entanglement molecular weight, Ms >> Mw, is well entangled. When a thin polymer film is uniaxially strained below the glass transition temperature crazes are formed. Measurements of the volume fraction of the deformed versus the undeformed framework. [1] X. Mao, P. M. Goldbart, X. Xing and A. Zippelius, Europhys. Lett. 80, 26004 (2007).

3:30PM S25.00006 Organogels from Polypeptide-based Block Copolymers, DANIEL SAVIN, DANIEL BERCOCI, SANDEEP NAIK, Department of Chemistry, University of Vermont — A series of AB diblock and ABA triblock copolymers consisting of poly(Lysine) (A) ( = P(Lys(Z)) ) and poly(propylene oxide) (B = PPO) were synthesized and found to form stable, rigid organogels in THF (ca. 1.5 wt.% solutions) at room temperature. In these systems, the protecting group on the P(Lys) side-chains remains intact. As such, the secondary structure of the polypeptide chains retains its helicity over a wide range of solution conditions. Gel formation in these systems results from the assembly of the solvethenphobic P(Lys(Z)) chains, which pack densely in an anti-parallel fashion, minimizing interfacial curvature. These gels exhibited shear-thinning behavior, and as the temperature was heated to 77°C exhibited a gel-sol transition. The gels formed over a time scale of about 10 minutes and had a modulus on the order of 55 Pa. The molecular weight dependence of the gel formation and rheological properties was studied in THF, dioxane and toluene.

3:42PM S25.00007 Soft random solids and their spatial elastic heterogeneity, XIAOMING MAO, PAUL GOLDBART, University of Illinois at Urbana-Champaign, XIANGJUN XING, Syracuse University, ANNETTE ZIPPELIES, University of Goettingen — As a consequence of the disorder that is quenched in at synthesis, random solids are spatially heterogeneous, not only in their structure but also in their response to external conditions. For the case of soft random solids, the heterogeneity in the elasticity is particularly intriguing, owing to its entropic origin and the interplay with incompressibility. We have examined the issue of heterogeneity in the elastic properties of soft random solids by applying replica statistical mechanics to a semi-microscopic model of a random network medium [1]. We have characterized the elastic heterogeneity by random residual stress and Lame coefficient fields, and have determined the statistics of these quantities. We have found that correlations involving the residual stress field are long ranged, and are governed by a universal parameter that also determines the mean shear modulus. Non-affine elastic deformations in soft random solids can also be also studied within this framework. [1] X. Mao, P. M. Goldbart, X. Xing and A. Zippelius, Europhys. Lett. 80, 26004 (2007).

3:54PM S25.00008 Effective removal of entanglement points by network dilution, JOSHUA D. MCGRAW, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — A polymer system in which the chains are much longer than the entanglement molecular weight, Ms >> Mw, is well entangled. When a thin polymer film is uniaxially strained below the glass transition temperature crazes are formed. Measurements of the volume fraction of the deformed versus the undeformed regions can give information on the entanglement density of the system[1]. We present results of such deformation experiments, probing using atomic force microscopy, in which well entangled networks have been diluted with chemically identical species of molecular weight, Mw << Ms, which results in a decrease in the entanglement density. Varying the length of the diluted chains provides molecular information on how the entanglement network is swollen.


4:06PM S25.00009 Advances in elastomer reinforcement: slow dynamics, PAUL SOTTA, CNRS/Rhodia Research and Technology, France, STÉPHANE DUPRES, PIERRE-ANTOINE ALCOUY, CNRS/university Paris-Sud, Orsay, France, DANIEL LONG, CNRS/Rhodia Research and Technology, France — Elastomers reinforced with nanometric solid particles or aggregates exhibit remarkable properties which are still far from being completely understood: reinforcement, non linear effects, irreversibility. Important progress has been achieved recently in modeling these properties, based on glassy layers around filler particles. In some cases, reinforcement as a function of temperature and filler volume fraction was explained quantitatively. We shall present an ensemble of experimental results obtained in various filled elastomers, which give some new insight on the microscopic mechanisms of reinforcement. We shall focus on two aspects: local strain measured by combining various techniques (NMR, mechanics, onset of strain-induced crystallization), indicate the level of stress heterogeneity in the elastomer matrix in the presence of reinforcing fillers; slow relaxation phenomena which occur in these systems: stress relaxation, memory effects and irreversibility effects -such as plasticity- indicate the importance of glassy regions within the matrix. Refs: J Berriot et al., Europhys. Lett. 2003, 64, 50-56; D. Long and P. Sotta, Macromolecules 2006, 39, 6282.

4:18PM S25.00010 Polydomain-Monodomain Transition of Randomly Disordered Nematic Elastomers with Different Crosslinking Histories, KENJI URAYAMA, ETSUKO KOHMON, RYO MASHITA, TOSHIKAZU TAKIGAWA, Kyoto University — When the mesogenic molecules (polymers) are crosslinked without a special care for global alignment, the resultant networks have a polydomain structure with local orientational order (in the order of micron) but without macroscopic order. It is well known that such polydomain liquid crystal elastomers (PLCE) exhibit a transition to the monodomain state with global orientation under a finite stretching stress. In present study, we examine the polydomain-monodomain (PM) transition of the two types of PLCE (I-PLCE and N-PLCE) that are originally formed in the high-temperature isotropic or low-temperature polydomain nematic states. They show no appreciable difference in the equilibrium properties such as transition temperature and swelling degree. In contrast, their transition behaviors are significantly different: The transition in I-PLCE occurs sharply at a critical stress whereas that in N-PLCE proceeds gradually over a wide range of stress.
4:30PM S25.00011 New Insights Regarding the Polydomain-to-Monodomain Transition in Smectic Elastomers1, RONALD HEDDEN, HARSHAD PATIL, DANIEL LENTZ, Penn State University — Smectic elastomers are rubber-like networks characterized by lamellar mesophases. Crosslinking a smectic polymer in the absence of an aligning field produces a polydomain elastomer containing numerous randomly oriented microdomains. Under uniaxial tension, polydomain smectic elastomers undergo a transition to a globally oriented “monodomain” state, which may proceed by rotation and/or transient disordering of microdomains. New studies of smectic main-chain elastomers suggest that disordering of microdomains via unfolding of hairpin structures is the dominant mechanism for elongation at intermediate strains. A “plateau stress” is found in plots of the nominal stress vs. strain, which correlates with the average domain size. At very high strains, elastic chains approach the finite extensibility limit, and layer buckling becomes the predominant mechanism for elongation. The elongation mechanism differs significantly from that in mesomorphic poly(diethyldisiloxane) elastomers, which also exhibit a “plateau” in the nominal stress vs. strain curve due to spontaneous random coil-to-helix transition. Because of chain-folding in main-chain smectics, the P-M transition may exhibit some similarities with the cold drawing of semicrystalline polymers.

1Supported by U.S. National Science Foundation grant DMR-0733658.

4:42PM S25.00012 Nematic elastomers: From a microscopic model to macroscopic elasticity theory, PAUL GOLDBART, University of Illinois at Urbana-Champaign, XUANGJUN XING, Syracuse University, STEPHAN PFÄHL, University of Mainz, SWAGATAM MUKHOPADHYAY, Rutgers University, ANNETTE ZIPPELIUS, University of Goettingen — A Landau theory is constructed for the gelation transition in cross-linked polymer systems possessing spontaneous nematic ordering, based on symmetry principles and the concept of an order parameter for the amorphous solid state. This theory is substantiated with help of a simple microscopic model of cross-linked dimers. Minimization of the Landau free energy in the presence of nematic order yields the neo-classical theory of the elasticity of nematic elastomers and, in the isotropic limit, the classical theory of isotropic elasticity. These phenomenological theories of elasticity are thereby derived from a microscopic model, and it is furthermore demonstrated that they are the universal mean-field descriptions of elasticity for all chemical gels and vulcanized media.

4:54PM S25.00013 Elasticity of a Chiral elastomer, APRANA BASKARAN, XUANGJUN XING, Syracuse University — We study the nonlinear elasticity of an elastomer made by crosslinking a chiral polymer melt in its isotropic state. It is shown that such an elastomer is unstable to uniaxial extension/compression and tends to develop a twist along the axis of deformation. Both phonon correlation functions and polarization dependent sound velocity are calculated. Furthermore, when such an elastomer is cooled below the isotropic-nematic transition of the underlying polymer melt, it develops inhomogeneous spontaneous deformations to accommodate the emergent chiral ordering of the polymers. We perform variational analysis of these spontaneous deformation in different regimes of system parameters.

5:06PM S25.00014 Determination of the refractive indices of liquid crystal elastomers1, ISRAEL LAZO, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — Liquid Crystal Elastomers (LCEs) are fascinating materials due to the coupling between orientational order and mechanical strain. We investigate this coupling by studying the optical properties of LCEs. We have measured the ordinary and extraordinary refractive indices of nematic LCEs as function of strain using two different techniques. In both cases, the strain is applied along the nematic director. The first technique is a Brewster’s angle measurement which is based on reflection of the incident light and the second is a conoscopic Mach-Zehnder interferometer based on transmission. We present our experimental results and methods of analysis. We compare our observations with theoretical predictions.

1This work was supported by the NSF under grant DMR 0606357.

5:18PM S25.00015 Magnetooactive Liquid Crystal Elastomers, MORITZ WINKLER, Heinrich Heine Universitaet Dusseldorf, ANDREAS KAISER, Heinrich Heine-Universitaet Dusseldorf, SIMON KRAUSE, HEINO FINKELMANN, Albert Ludwigs-Universitaet Freiburg, ANNETTE SCHMIDT, Heinrich Heine-Universitaet Dusseldorf, DUESSELDORF TEAM, FREIBURG TEAM — Liquid crystal elastomers (LCEs) offer an interesting spectrum of properties, including temperature induced, fully reversible shape changes connected with considerable development of pulling force, and synthetic diversity. In order to take advantage of LCEs for an extended number of viable devices, it is desirable to trigger such shape changes with electromagnetic fields rather than temperature changes. Magnetooactive LCEs are accessible by the incorporation of superparamagnetic Fe3O4 nanoparticles into oriented nematic side-chain LCEs and offer a contactless activation pathway to activate the nematic-to-isotrope transition by local magnetic heating in external fields due to relaxation processes. In magnetomechanical measurements at 300 kHz and 43 kA m−1, a sample contraction of up to 30 % is observed under field influence, that is fully released when the field is switched off. The load evolved reaches 60 kPa and more. The materials’ ability to respond to a contactless electromagnetic stimulus with a well-defined contraction can be of use for various actuator applications.

5:30PM S25.00016 Calamatic liquid crystal elastomers swollen with bent-core liquid crystals, M. CHAMBERS, Liquid Crystal Institute, Kent State University, Kent, OH, J.T. GLEESON, S. SPRUNT, Department of Physics, Kent State University, Kent OH, A. JAKLI, Liquid Crystal Institute, Kent State University, Kent OH. — Liquid crystal elastomers are composed of a chemically bonded liquid crystal mesogen and an elastomeric polymer network. They exhibit both the properties of rubber elasticity, liquid crystallinity and their interplay, giving rise to unique systems rich in physics. Additionally, bent-core ("banana") liquid crystals are also of interest exhibiting rich phase behaviour and non-classical properties such as flexoelectricity. Here we examine the swelling of calamatic liquid crystal elastomers with various bent-core mesogens and the intriguing properties of the resulting system. The consequential swollen liquid crystalline elastomer systems, can imbibe many times their weight and volume in bent core mesogens until saturated. The homogenous system displays new properties (transition temperatures and phases) depending strongly on the interaction of the elastomer mesogen and bent-core mesogen. Strangely, for some bent-core mesogens this leads to higher temperature phase behaviour than both compounds originally possess. The authors would like to acknowledge support from ONR (N00014-07-1-0440) and NSF (DMR-0606160).

Wednesday, March 12, 2008 2:30PM - 4:54PM — Session S26 DCP: Focus Session: Advances in Atmospheric Aerosol Science — Morial Convention Center 218
2:30PM S26.00001 Tropospheric Aerosol Chemistry via Aerosol Mass Spectrometry. DOUGLAS WORSNOP, Aerodyne Research, University of Helsinki — A broad overview of size resolved aerosol chemistry in urban, rural and remote regions is evolving from deployment of aerosol mass spectrometers (AMS) throughout the northern hemisphere. Using thermal vaporization and electron impact ionization as universal detector of non-refractory inorganic and organic composition, the accumulation of AMS results represent a library of mass spectral signatures of aerosol chemistry. For organics in particular, mass spectral factor analysis provides a procedure for classifying (and simplifying) complex mixtures composed of the hundreds or thousands of individual compounds. Correlations with parallel gas and aerosol measurements (e.g. GC/MS, HNMR, FTIR) supply additional chemical information needed to interpret mass spectra. The challenge is to separate primary and secondary, anthropogenic, biogenic and biomass burning sources and subsequent transformations of aerosol chemistry and microphysics.

In collaboration with: Tim Onasch, Manjula Canagaratna, John Jayne, Jesse Kroll, Achim Trimborn, Aerodyne Research; Ingrid Ulbrich, Allison Aiken, Peter DeCarlo, Jose Jimenez University of Colorado; Qi Zhang, SUNY Albany.

3:06PM S26.00002 The Dynamic Interaction of Chemistry and Phase Partitioning in Atmospheric Organic Aerosols. NEIL DONAHUE, Carnegie Mellon University — Atmospheric organic aerosols are a dynamic, chemically evolving mixture in equilibrium between the gas and condensed phases. This applies equally to primary emissions, which span a huge range in volatility, as well as secondary oxidation products generated by chemical reactions in both phases. The degree of volatility of primary emissions has been historically underappreciated, and the role of oxidation reactions has been considered in almost all cases only through their first or two generations. We have recently developed a ‘volatility basis set’ to address both primary volatility distributions and secondary volatility evolution (sometimes called primary organic aerosol and secondary organic aerosol). Here we will discuss both facets of this framework and apply to organic aerosols on all scales, from emissions measurements to global organic aerosol loadings. We shall describe ongoing experimental work to constrain volatility distributions and volatility evolution through chemistry as well as extensions to the basis-set framework to more fully describe evolving aerosol properties.

In collaboration with Allen Robinson, Carnegie Mellon University.

3:42PM S26.00003 Tandem mass spectrometry of single organic aerosol particles: A promising approach for in-situ analysis of mixtures. PEDRO CAMPUZANO JOST, SARAH HANNA, EMILY SIMPSON, DAMON ROBB, MICHAEL BLADES, JOHN HEPBURN, ALLAN BERTRAM, University of British Columbia — We have built a new single particle mass spectrometer for organic aerosol analysis that combines different previously tried approaches into one single instrument. We use soft, wavelength tunable desorption by using a dedicated pulsed CO2 laser, (Prather, Baer & coworkers) and soft ionization by tunable VUV radiation (Baer, Wilson & coworkers)) to ensure a minimum of fragmentation. By ionizing the aerosol plume in the center of an ion trap both high sensitivity and the ability to elucidate structure by tandem mass spectrometry (Reilly & coworkers) can be achieved. The analytical performance of the instrument as well as the detection geometry has first been validated by using simple ionization techniques, 70 eV El and REMPI, on a suite of aromatic and aliphatic compounds and simple mixtures. The novel tunable VUV laser system has been thoroughly characterized with a host of gaseous organic compounds that has proven both the ability to determine ionization energies with high accuracy and the possibility in many cases to minimize fragmentation by tuning the VUV source close to the ionization threshold. The VUV source has been integrated into the aerosol mass spectrometer and first VUV single aerosol spectra will be presented.

3:54PM S26.00004 A novel flow reactor for studying the hydrolysis of N2O5 on aqueous H2SO4 solutions coated with organic surfactants. DANIEL KNOPP, Institute for Terrestrial and Planetary Atmospheres, Stony Brook University, LORI COSMAN, ALLAN BERTRAM, Dept. of Chemistry, UBC, PAYAM MOUSAVI, SATYA MOKAMATI, Dept. of Mech. Eng., UBC — A flow reactor has been developed which allows the study of heterogeneous kinetics on an aqueous surface coated by organic monolayers. Computational fluid dynamics simulations have been used to determine the flow characteristics for various experimental conditions. A mathematical framework has been developed which allows the study of heterogeneous kinetics on an aqueous surface coated by organic monolayers. Computational fluid dynamics simulations have been used to determine the flow characteristics for various experimental conditions. A mathematical framework has been developed which allows the study of heterogeneous kinetics on an aqueous surface coated by organic monolayers. Computational fluid dynamics simulations have been used to determine the flow characteristics for various experimental conditions. A mathematical framework has been developed which allows the study of heterogeneous kinetics on an aqueous surface coated by organic monolayers. Computational fluid dynamics simulations have been used to determine the flow characteristics for various experimental conditions.
2:30PM S27.00001 Probing Magnetic Nanostructures on the Atomic Scale. CYRUS F. HIRJIBEHELIN, London Centre for Nanotechnology, Deps. of Physics & Astronomy and Chemistry, University College London — Magnetic nanostructures are increasing data storage capacities and are promising candidates for implementations of novel spin-based computation techniques. The relative simplicity and reduced dimensionality of nanoscale magnetic structures also make them attractive model systems for studying fundamental interactions between quantum spins. We used a scanning tunneling microscope to build individual magnetic nanostructures one atom at a time. By measuring their spin-excitation spectra with inelastic electron tunneling spectroscopy, we determined the orientation and strength of the anisotropies of individual Fe and Mn atoms on copper nitride. First-principles calculations indicate that the magnetic atoms become incorporated into a polar covalent surface molecular network, making them similar to the building blocks of magnetic rare earths. In linear chains of up to 10 Mn atoms, we observed excitations of the coupled atomic spins that can change both the total spin and its orientation. The large magnetic anisotropy and strong spin-coupling manifested in these structures, which provide atom-by-atom accessibility via local probes, have the potential to produce atomic-scale magnetic structures that have a stable magnetization at low temperatures.

* This work was done in collaboration with C.-Y. Lin, A.F. Otte, M. Ternes, C.P. Lutz, B.A. Jones, and A.J. Heinrich at the IBM Almaden Research Center, San Jose, CA 95120 USA.

3:06PM S27.00002 Initial Metallization and Transition Metal Diffusion in ZnO Single Crystals, CVD-Grown Films, and Nanostructures. SENIA KATALINIC, SYLVIE RANGAN, RODNEY GATEAU, PAN WU, YICHENG LU, ROBERT BARTYNSKI, Rutgers University — Transition metal doped ZnO is a promising candidate room temperature dilute magnetic semiconductor for spintronic applications. In previous studies indicate Fe or Mn dopants exhibit significantly different diffusion properties in ZnO. To explore whether this is an inherent property of ZnO or if it is related to non-related aspects of the films or nanostructures, we have studied the initial stages of Mn, Fe, and Cu metallization of the single crystal ZnO(0001)[Zn-terminated] and (11-20) surfaces, as well as MOCVD-grown epitaxial a-plane films using scanning tunneling microscopy and spectroscopy (STM and STS). While deposited Cu forms well defined islands, all three surfaces exhibit substantial disruption upon Fe deposition, including significant change in terrace widths and a markedly smaller fraction of atomic height steps. Upon annealing, Cu islands become mobile and coarsen, but the underlying ZnO structure is not strongly affected. Annealing with Fe on the surface, significant coarsening and roughening of the substrate occurs even at the modest annealing temperature of 200°C, and this effect is enhanced upon annealing to 400°C. Initial results suggest that uptake of metals into the epi-film is predominantly determined by the properties of the (11-20) surface that terminates the film.

3:18PM S27.00003 Unusual size-dependent magnetic anisotropy in Co nanomagnets made from self-organized fast laser processing1, H. KRISHNA, Dept. of Physics, Washington University in St. Louis, MO, C. MILLER, Dept. of Electrical and Systems Engineering, Washington University in St. Louis, MO, Z. NUSSINOV, A.K. GANGOPADHYAY, R. KALYANARAMAN, Dept. of Physics, Washington University in St. Louis, MO — Unusual size-dependent magnetic anisotropy has been observed in hemispherical polycrystalline Co nanomagnet on SiO2 substrates produced by fast pulsed-laser-induced self-organization. The magnetic states of these particles have been characterized by using magnetic force microscopy (MFM) and hysteresis measurements. The results for single domain particles up to a diameter of 180 nm, the magnetization direction of smaller sized particles tends to be in-plane, while the larger particles tend to have out-of-plane orientation. This finding is not consistent with shape anisotropy which predicts a size-independent in-plane alignment. Microstructural analysis revealed that particles had a granular microstructure with the grain size increasing with particle size. This unusual behavior has been attributed to large residual tensile strain in the hemispherical nanoparticles due to the large heating/cooling rates (∼1010 K/s) under ns laser self-organization, the large thermal expansion mismatch and the negative magnetostricitive constant for polycrystalline Co.

1This work was supported by a Center for Materials Innovation grant # 94509A to AKG and RK and by the National Science Foundation through CAREER grant # DMI-0449258 to RK.

3:30PM S27.00004 Magnetocaloric effect (MCE) in ferrite nanoparticles1, JAMES GASS, HARIHARAN SRIKANTH, University of South Florida — Enhancement of the magnetocaloric effect (MCE) in nanostructured materials is important for refrigeration applications particularly in potential spot cooling of MEMS and NEMS devices. We have investigated MCE in various classes of polydisperse and monodisperse soft ferrite nanoparticles with different blocking characteristics. Our observations indicate that in some systems, surface properties such as spin disorder and anisotropy lead to considerable enhancement of MCE. This is promising for potentially increasing MCE in nanoparticle systems through systematic engineering of the surfaces via core-shell or other approaches. We report on the magnetocaloric effect (MCE) in several ferrite nanoparticle systems and compare them. Characterization of structural and magnetic properties was done using XRD, TEM, DC and AC magnetization, and transverse susceptibility. The change in entropy was calculated using the thermodynamic Maxwell relation from the family of M-H curves taken at different temperatures. The specific role of surface anisotropy and surface structure in ferrite nanoparticles and correlation to the MCE will be discussed.

1Work at USF supported by a grant from DOE-BES

3:42PM S27.00005 A magnetic nanoparticle as an ultimate voltage-controlled nanomagnet1, IGOR OVCHNIKOV, E&E Dept. UCLA, KANG WANG, E&E Dept. UCLA, FENA, WIN, CNSI — We argue that when the conduction band edge of a semiconductor is aligned with the Fermi level, the valence band states have a high probability of being occupied. By controlling the voltage on the semiconductor surface, we can control the occupation of these states and thus control the magnetization of a magnetic nanoparticle. This concept is demonstrated using ZnO nanocrystals grown on Si substrates. The nanocrystals are grown using a self-organized wet chemical method and are characterized by scanning tunneling microscopy and spectroscopy (STM and STS). The nanocrystals are then functionalized with a magnetic layer, and the magnetic properties are measured using magnetic force microscopy (MFM) and hysteresis loops. The results show that the magnetic properties of the nanocrystals are highly dependent on the voltage applied to the semiconductor surface. This work is supported by the NSF and DOE.

1The work was partly supported by FENA and WIN.

3:54PM S27.00006 Anisotropy-Compensated Magnetic Nanostructures1, RALPH SKOMSKI, TOM ALGER, GEORGE, D.J. SELLMYER, NCMN and Dept. Physics & Astronomy, University of Nebraska — Nanostructuring can be used to tailor the magnetic anisotropy K1 as function of temperature, which is important in permanent magnetism and magnetic recording. Anisotropy is an atomic quantity, but the ferromagnetic exchange ensures an anisotropy averaging over a few nanometers, in contrast to the absence of nanoscale Curie-temperature averaging [1]. An intriguing and largely overlooked feature is the possibility of temperature-dependent anisotropy zeros, which yields a potential write-field reduction in magnetic recording. On an atomic scale, this effect is well-known but limited to a relatively narrow range of rare-earth transition-metal intermetallics. Nanostructuring greatly extends the range of materials. Explicitly considered materials are thin films, where the determination of the anisotropy zero (s) yields algebraic equations whose roots depend on the thicknesses, Curie temperatures, and zero-temperature anisotropies of the involved phases. On a somewhat larger length scale (j 5 to 10 nm), there is no longer a well-defined anisotropy, but the corresponding micromagnetic corrections are easily incorporated into the theory. - [1] R. Skomski, “Simple Models of Magnetism,” University Press, Oxford 2008.

1This research is supported by NSF MRSEC and INSIC.
4:06PM S27.00007 Lattice Induced Configurational Anisotropy in Nanomagnets\textsuperscript{1} 1, WEN ZHANG, NOAH BRAY-ALI, STEPHAN HAAS, University of Southern California — The study of magnetic nanoparticles is evolving into a rich and rapidly growing area, featuring many novel phenomena and potential applications. One of the most important properties of these systems is the magnetic anisotropy, which determines the blocking temperature. Besides the well-known crystalline and shape anisotropies, the competition of exchange and magneto-static interactions in nanomagnets leads to the formation of a configurational anisotropy, resulting from small deviations of the magnetization from uniformity within the nanostructures. In this talk, I discuss a new type of anisotropy, i.e. the lattice induced configuration anisotropy, which we have studies using Monte Carlo simulations. In particular, a scaling approach has been shown to be effective in obtaining the magnetic properties of nanoparticles. The relationship between anisotropy and blocking temperature will also be discussed. Understanding the influence of anisotropy opens up a new path to designing nanostructured magnetic materials with novel functionalities.

\textsuperscript{1}We acknowledge USC high-performance supercomputing center and financial support by the Department of Energy under grant DE-FG02-05ER46240.

4:18PM S27.00008 Between ferro- and para-magnetism. Electron magnetic resonance and quantal effects in superparamagnetic nanoparticles, NATALIA NOGINOVA, Norfolk State University, Norfolk VA, MAXIM NOGINOV, Cornell University, Ithaca, NY, VADIM A. ATSarkin, IRE, Moscow, Russia — Nanometer-scale magnetic objects are at the interface between quantum dynamics of several interacting spins and classical thermodynamics of multi-particle systems. We present results of electron magnetic resonance (EMR) studies in suspensions of two different systems with superparamagnetic iron oxide nanoparticles with average size of 5 nm and 9 nm correspondingly. It is shown that both types of particles demonstrate common EMR behavior, including the broad spectral component, temperature-dependent narrow component with g-factor of $\sim 2$, and additional low-field signals observed at the fields $B_{\text{B1}} = B_0/k$, where $B_0$ is the resonance field of the main resonance, and $k = 2, 3$, and 4. These lines correspond to the transitions at the double, triple, etc., resonance frequencies and can be described in terms of the non-secular spin operators arising from the single-particle magnetic anisotropy or inter-particle dipole-dipole interactions. These features are common for small quantum systems and not expected in classical case. The relative intensity of the narrow component and low-field signals rapidly decreases with cooling or increase of particle size, marking gradual transition to classical FMR behavior.

4:30PM S27.00009 Finite size effect in shell nanoparticles, JOSHUA KOCH, RENAT SABRIANOV, University of Nebraska Omaha — The magnetic properties of single layer shell particles studied as function of the particle’s size using Monte Carlo method with free boundary conditions. We formed truncated octahedron shell-nanoparticles of 4-30 lattice spacings across mimicking particles from 2-12 nm in size. The classical Heisenberg model with nearest neighbor ferromagnetic (FM) and antiferromagnetic (AFM) exchange interactions shows the existence of the well defined ground state. FM nanoparticles have susceptibility maximum decreasing with the increase of the nanoparticle size. Finite size scaling analysis predicts small Curie temperature for shells of the large size. The AFM particles built as truncated octahedron with (001) and (111) planes of the cubic lattice show freezing in the noncollinear structure with very low magnetization. The freezing temperature determined as maximum in specific heat in particles with AFM does not change strongly with the size of the shell in the studied particle sizes. We clearly observe the effects of edges and corners on the properties of shell particles resulting in deviation from simple scaling behavior. We fit the size dependence variation of thermodynamic properties maxima using the idea of the continuous dimensionality and the fact that infinite 2D systems do not exhibit long range order at finite temperature in the continuous symmetry.

4:42PM S27.00010 Low T magnons condensation in FePd and FePt nano-particulate films, R. A. LUKASZEW, K. YANG, J. R. SKUZA, C. CLAVERO, The College of William and Mary, VA — Recently there have been interesting reports on experimental deviations from the Bloch T$^{3/2}$ law at low temperature in magnetic nanostructures. Specifically it has been reported an “upturn” of the T$^{3/2}$ law in the magnetization in some nanomagnetic materials. [1] This behavior has been attributed to a Bose-Einstein Condensation of magnons in the nanostructured materials due to more disorder in the spins at finite entropy as opposed to the case of crystalline bulk ferromagnets where it can be assumed that all the spins are in the direction of a saturating magnetic field and hence perfectly ordered. In order to further test these ideas, we have carried out systematic low temperature magnetization studies (SQUID) on FePd and FePt nano-particulate thin films. The microstructure and morphology of the thin films have also been extensively characterized with X-Ray, TEM and AFM/MFM. We will show our experimental data and point out significant differences and also similarities in the analyzed samples. [1]. Extension of the Bloch T$^{3/2}$ Law to Magnetic Nanostructures: Bose-Einstein Condensation, E. Della Torre, L. H. Bennett and R. E. Watson, Phys. Rev. Lett. 94, 147210 (2005).

4:54PM S27.00011 Strong-field interactions between a nanomagnet and a cavity mode, O. SOYKAL, M. E. FLATTE, OSTS and Department of Physics and Astronomy, University of Iowa — We analyze the interaction of a nanomagnet with a single mode of a microcavity in a fully quantum-mechanical treatment. We consider a spherical cavity roughly 1 mm\textsuperscript{3} in volume, and a nanomagnet consisting of 10\textsuperscript{10} spins treated as a macrospin, in the presence of a static magnetic field. For an initial configuration of no photons in the cavity and the macrospin oriented antiparallel to the field, the interaction Hamiltonian contains magnet-microwave mode coupling terms that exceed several GHz. Thus for quality factors in excess of 100, strong-field effects should be observable in the nanomagnet/cavity dynamics. Coherent states of the nanomagnet/photon system are characterized by large oscillations in the photon number (and nanomagnet spin), and are characterized by exceptionally long dephasing times.

3This work was supported by an ONR MURI

5:06PM S27.00012 Magnetism of Fe double wires deposited on Ir(100), RICCARDO MAZZARELLO, SISSA, Trieste, Italy, ANDREA DAL CORSO, SISSA and DEMOCRITOS-INFM, Trieste, Italy, ERIO TOSATTI, SISSA, ICTP and DEMOCRITOS-INFM, Trieste, Italy — Bulk bcc Fe is a prototypical ferromagnet (FM), but a single monolayer of Fe on W(001) has been known to be antiferromagnetic (AFM). Very recent spin-polarized STM experiments on Fe double chains deposited on Ir(100) 5x1 [1] showed that these adsorbed nanowires are AFM too [2]. We study the magnetic properties of this system using ab-initio density functional theory and both scalar-relativistic and fully-relativistic ultrasoft pseudo-potentials. In particular, we address the energetics of FM and AFM configurations of several experimentally relevant structures. The AFM configuration is always energetically favored, which is in agreement with experiment but does not yet allow to distinguish between different structures. Investigation of the magnetic anisotropy induced by the spin-orbit interaction is in progress. [1] L. Hammer, W. Meier, A. Schmidt, and K. Heinze, Phys. Rev. B 67, 125422 (2003). [2] R. Wiesendanger, private communication.

5:18PM S27.00013 Tailoring magnetic order in nanowires by alloying 5d Transition Metal elements, JAVIER GUEVARA, Escuela de Ciencia y Tecnologia-UNAMS e INN-CNEA, TRISTANA SONDON, Departamento de Fisica e INN-CNEA, ANDRES SAUL, CRM CNRS, Marseille, Francia — The magnetism of pure-element nanowires have been theoretically studied and show, in the case of Au, Pt, and Ir, nanomagnets with anisotropic magnetic properties of A$_1$, B$_2$, C$_3$; nanowires being A$_1$, B$_2$, O$_3$, Ir, or Pt, by using the ab-initio Wien2k code. These alloyed nanowires have large magnetic moment values, and also giant MAE of different signs. We show the evolution of the spin and orbital magnetic moments as the magnetization axis is being varied.
2:30PM S28.00001 Design of uniaxial metallodielectric metamaterials having large optical nonlineairities. JOSEPH GEDDES, ERIK NELSON, PAUL BRAUN, University of Illinois at Urbana-Champaign — We describe how the intrinsically large optical nonlinearities of metals could be accessed and increased by fabrication of uniaxial homogenized composites comprising alternating metal and dielectric layers of subwavelength thickness. Such composites are predicted to exhibit effective third-order nonlinear susceptibilities of magnitude larger than those intrinsic to the metallic component. The enhancement is due to a resonance effect, and is limited to the direction perpendicular to the layer interfaces. We illustrate our predictions with calculations for several metallodielectric systems, including those consisting of copper and titanium dioxide components.

2:42PM S28.00002 Spectroscopic and thermal studies of L-arginine doped Potassium Dihydrongen Phosphate crystals. JAYESH GOVANI, FELICIA MANCIU, Department of Physics, University of Texas at El Paso, El Paso, TX 79968, U.S.A, MIHIR JOSHI, KETAN PARIKH, DIPAK DAVE, Department of Physics, Saurashtra University, Rajkot, Gujarat-360 005, India — We have used IR transmission and Raman spectroscopy to study the active doping of potassium dihydrogen phosphate (KDP) crystals with L-arginine amino acid. In the present investigation, pure and doped KDP crystals were grown by slow evaporation solution method. Although the dominant bands observed in the infrared absorption spectra correspond to KDP crystals, the existence of vibrational lines at 1401 cm⁻¹ (CH₂), 1637 cm⁻¹ (COO⁻), 1716 cm⁻¹ (NH₃⁺), and 3127 cm⁻¹ (NH₄⁺) indicate that successful doping was achieved. This affirmation is further corroborated by the FT-Raman data, where strong lines are observed in the 2800 cm⁻¹ – 3100 cm⁻¹ region, which is associated with C-H stretching modes of amino acids. The crystal structure and the thermal stability of the samples were also examined by powder X-ray diffraction and thermogravimetric techniques, respectively. Thermogravimetric analysis demonstrates a decrease of the thermal stability with increasing doping amount. An increase of second harmonic generation efficiency was found with more L-Arginine doping.

2:54PM S28.00003 Optical properties in the visible range of Co clusters capped by Pd under hydrogen. 1. A.L. CARRERA, J.I. AVILA, Facultad de Fisica, Pontificia Universidad Catolica de Chile, C.P. ROMERO, M.J. VAN BAEL, P. LIEVENS, Laboratorium voor Vaste-Stofsysca en Magneteisme, Katholieke Universiteit Leuven — Co clusters with mean size of 1.8 nm were deposited to form a 25 nm thick cluster assembled film on glass, capped by a continuous 15 nm Pd film. The light transmission and reflection, in the visible range (400 to 1000 nm), were measured when the sample was exposed to different hydrogen pressures up to 120 Torr. Measurements on 15 nm continuous Pd film were done for comparison. Electrical resistance of the films was also measured as an independent parameter to determine hydrogen absorption by the samples. In both samples the transmission and resistance of the films increase, reaching saturation at 30 Torr hydrogen pressure. Increase of the light transmission and electrical resistance on the pure Pd film indicates absorption of hydrogen in the bulk of the film. Smaller relative change of the resistance and reflection of light on the Co cluster sample capped by Pd indicates that hydrogen absorption is limited to the Pd capping layer only. This work is supported by the Fund for Scientific Research-Flanders (FWO), by the Flemish Concerted Action (GOA), and by the Belgian Interuniversity Poles of Attraction (IAP) programs.

3:06PM S28.00004 Novel optical signatures of sub-3 nm rare earth sesquioxide nanocrystals. JAMES DICKERSON, Department of Physics and Astronomy, Vanderbilt University, Nashville TN, SAMEER MAHAJAN, Interdisciplinary Program in Materials Science, Vanderbilt University, Nashville, TN — Europium and terbium based sesquioxide nanomaterials, known for their characteristic red and green luminescence, respectively, have recently garnered much research attention due to their size-dependent optical properties. Here, we present systematic investigation of the size-dependent optical properties Eu₂O₃, Tb₂O₃, and Gd₂O₃Eu³⁺ / Tb³⁺ nanocrystals (NCs) in the size range of 1-3 nm in diameter. We observe a new luminescence peak at 620 nm in Eu₂O₃ and Gd₂O₃Eu³⁺ NCs, which represents modulation of the 5F₂ transition in Eu³⁺ ion. Intensity modulation with respect to the 612 nm is observed as a function of nanocrystal size. For the Tb₂O₃ NCs, a new luminescence signature at 548 nm characterizes modulation of the 5F₄ transition in Tb³⁺ ion. In addition, we probe the effect of NC size on the luminescence efficiencies of the doped and pure sesquioxide NCs. The concentration quenching effect, which leads to low luminescence efficiencies in bulk, pure sesquioxides, is explored in sub-3 nm sesquioxides.

3:18PM S28.00005 Far-infrared Magneto-Spectroscopic Studies of Ca₃CoO₄ Thin Films and Single Crystals. 1 JIUFENG TU, DAMITR DIMITROV, CCNY, WEIDONG SI, QIANG LI, BNL — In recent years, the 2D-layered cobaltates have emerged as promising p-type thermoelectric materials due to their unique combinations of high thermo-coefficient and good metallic transport properties. These systems show high thermoelectric figure of merit and are ideal candidates as the materials of choice at elevated temperatures. We have carried out far-infrared magneto-spectroscopic studies of Ca₃CoO₄ thin films in Faraday geometry as a function of frequency, magnetic field and temperature with the emphasis on the coupling between the lattice, the charge and the spin degrees of freedom. Far infrared transmission reduces at low frequencies in the presence of magnetic field corresponding to negative magneto-resistance. Below 20K, hysteresis occurs. However, the spectral responses to magnetic field and temperature are different. This indicates that the negative magneto-resistance is due to reduced magnetic scattering when Co spins become aligned. Further infrared studies will be performed with magnetic field parallel to the CoO₄ layers. A good understanding of our infrared results should shed light on the origin of high thermo-power in these 2D-layered cobaltates.

3:30PM S28.00006 Ultrafast Time Resolved Transient Absorption and Photoluminescence (PL) Studies of In₅₀Ga₅₀As/GaAs Quantum Wells in High Magnetic Fields. 1 JINHO LEE, X. WANG, D.H. REITZIE, Physics Dept., University of Florida, S. MCGILL, NHMFL, Y.D. JHO, Dept. of Information and Communications, GIST, J. KONO, Dept. of Electrical and Computer Engineering, Rice University, A.A. BELYANIN, Physics Dept., Texas A&M University, G. SOLOMON, NIST — We investigate the temporal dynamics of dense magneto-plasmas excited by intense femtosecond laser pulses in In₅₀Ga₅₀As/GaAs multiple quantum wells in high magnetic fields. To fully fill the Landau levels (LLs), we pump to carrier densities near 10¹³ cm⁻² using 150 fs pulses. Time-resolved transient absorption experiments probe the occupancy of each e₁h₁ LL, revealing a dramatic decrease in decay times above the zero field e₁h₁ transition dynamics. Our PL results reveal evidence for multiple short bursts of emission pulses at the highest fields (17.5T) from in-plane PL emission compared with zero field emission. In addition, qualitatively different temporal dynamics from in-plane and out-of-plane collection geometries are observed. Our results are analyzed in the context of ultrafast cooperative emission mechanisms from dense electron-hole plasmas.

1 Supported by CUNY-RF-80299-11-13, DOE-AC02-98CH10886 and NSF-DMR-0451605.

1 Supported by the NSF through grant DMR-0325499 and by the NHMFL through an IHRP grant.
3:42PM S28.00007 Magneto-photoluminescence studies of CdTe/CdSe/ZnS nanoparticles. Y.H. CHANG, C.C. HUANG, L.W. CHANG, C.H. HSU, Department of Physics, National Taiwan University, CHIH-WEI LAI, CHIEN-LIANG LIU, PI-TAI CHOU, Department of Chemistry, National Taiwan University, Y.W. SUEN, Department of Physics, National Chung Hsing University — Recently, the effect of the magnetic flux on the excitonic energy has received much attention. Optical Aharonov-Bohm was observed on negatively charged exciton in InGaAs/GaAs quantum ring as well as neutral exciton in type-II InP-GaAs heterostructure. In this talk we will present our magneto-photoluminescence studies on the optical properties of CdTe/CdSe/ZnS system. The nanoparticles that were grown by chemical method have size of about 6 nm and the band alignment between the core (CdTe) and the shell (CdSe) is type-II band alignment. The addition of a ZnS layer is to passivate the surface of CdSe and to enhance the light emitting efficiency. Magneto-photoluminescence experiment was performed at T = 1.4 K with a 14 T superconducting magnet in conjunction with a green diode laser and a monochromator. Oscillation on the peak energy of the photoluminescence spectra as well as oscillation in the integrated intensity as a function of magnetic field were observed and are attributed to the optical Aharonov-Bohm-like effect.

3:54PM S28.00008 Absorption and photocurrent of semiconductor quantum wells: a multiband NEGF study. URS AEBERHARD, Paul Scherrer Institut — Interband photoexcitation of carriers in semiconductor quantum wells is exploited in various optoelectronic devices such as photodetectors or quantum well solar cells. For a quantitative prediction of the photocurrent, realistic models for the (sub)bandstructure as well as for the transport properties are required. In the present approach, the development of optical properties based on a multi-band empirical tight-binding Hamiltonian is combined with the non-equilibrium Green’s function formulation of quantum transport. The photocurrent is calculated in presence of elastic andinelastic electron-phonon scattering from the self-consistent Born approximation of the self energy for carrier-light interaction, while the absorption is obtained from the transverse interband polarization function. Since the absorption is observed experimentally by the excitonic contribution, the inclusion of this feature into the calculation of photocurrent and interband polarization via the respective many-body corrections is discussed.

4:06PM S28.00009 Magneto-infrared study on 2-dimensional electrons and holes in GaSb-InAs-AlSb coupled quantum wells. LI-CHUN TUNG, NHMFL, P.A. FOLKES, Army Research Laboratory, WEN XU, Australian National University, YONG-JIE WANG, NHMFL — InAs-AlSb heterostructures have been a subject of interests for their unusual type-II band alignment between InAs and AlSb. The spatially separated 2-dimensional electron and hole gases are confined in different layers and in equilibrium with each other at the InAs/GaSb interface. This unique circumstance has led to several predicted many-body effects, as well as possible applications as infrared detectors and sources. In the past, magneto-infrared studies on InAs-AlSb single quantum wells have revealed a range of phenomena arising from the electron-hole binding. We have carried out an infrared optical study up to 30T on a series of GaSb-InAs-AlSb coupled quantum well structures, in which the electrons and holes are separated by a thin barrier and the Fermi level is tuned by the thickness of the GaSb cap layer. In addition to the electron cyclotron resonance (CR), another transition has been observed at the fields higher than 13 T. The linewidth of the CR shows the oscillatory behavior with the filling factor that is consistent with the electron densities obtained from the transport measurements. The transition energy of this line is close to the energy difference between the lowest Landau level (LL) in the InAs layer and the highest LL in the GaSb layer, which suggests that the it might result from an excitonic transition across the barrier.

4:18PM S28.00010 Infrared dielectric properties and optical magnetoconductivity of CaRuO$_3$/CaMnO$_3$ superlattices. A.V. BORIS, P. YORDANOV, P. POPOVICH, B. KEIMER, Max Planck Institute for Solid State Research, Stuttgart, Germany, J.W. FREELAND, Argonne Nat. Lab., J. CHAKHALIAN, Univ. of Arkansas, Fayetteville, H.N. LEE, Oak Ridge Nat. Lab. — Spectroscopic ellipsometry and magneto-reflectivity in the far-infrared spectral range is used to study the electronic properties of [CaRuO$_3$]$_n$[CaMnO$_3$]$_{10n}$ superlattices (SLS). The nonlinear regression procedure is employed to extract the dynamical conductivity and dielectric permittivity of bare SLS within the effective medium approximation with a mixture of the ruthenate and manganite layers (N = 4-10 unit cells). This implies no major charge transfer effects between non-Fermi liquid metal CaRuO$_3$ and antiferromagnetic insulator CaMnO$_3$. While the low-energy electronic spectra of the SLSs is governed by CaRuO$_3$ layer behavior, we find a negative contribution, the inclusion of this feature into the calculation of photocurrent and interband polarization via the respective many-body corrections is discussed. The transition energy of this line is close to the energy difference between the lowest Landau level (LL) in the InAs layer and the highest LL in the GaSb layer, which suggests that the it might result from an excitonic transition across the barrier.

4:30PM S28.00011 Observation of coherent high-wavevector acoustic vibrations in a bulk material using time-resolved X-ray diffraction. MARIANO TRIGO, YU-MIIN SHEU, EMILY PETERSON, DAVID REIS, MATTHEW REASON, RACHEL GOLDMAN, ROBERTO MERLIN, University of Michigan, ERIC LANDAHL, Argonne National Laboratory, DONALD WALKO, DOHN ARMS, Argonne National Laboratory — We report on the observation of high-wavevector acoustic phonons in bulk InP that originate from folded phonons in the InAs layer and the highest LL in the GaSb layer, which suggests that the it might result from an excitonic transition across the barrier.

4:42PM S28.00012 Fröhlich phonon modes in PbSe and PbS colloidal quantum dots. JONATHAN WRUBEL, Harvard University, BYUNG-ROYOL HYUN, NIKOLAY AGLADZE, ALBERT SIEVERS, FRANK WISE, Cornell University — The measured infrared absorption of colloidal PbSe and PbS quantum dots in hexane is shown to be dominated by absorption near the Fröhlich mode frequency position. However, in both sets of quantum dots the mode is at a higher frequency than calculated from the bulk dielectric constant, and shifts to still higher frequency with decreasing diameter of dot. This behavior is shown to be consistent with a decreasing contribution of the near-infrared and visible exciton absorption to the dielectric constant at far infrared frequencies as the particle size decreases and the band gap increases. The unique presence of Fröhlich mode absorption in a wide range of dot sizes suggests that the mechanical boundary condition of the quantum dot is a “soft” one in which vibrational amplitudes do not go to zero at the boundary.

4:54PM S28.00013 Coherent defect-assisted multiphonon intraband carrier relaxation in semiconductor quantum dots. ALEXANDER PODDUBNY, Ioffe Institute, SERGUEI GOUPALOV, University of Utah & Ioffe Institute — A new defect-assisted mechanism of multiphonon intraband carrier relaxation in semiconductor quantum dots, where the carrier is found in a coherent superposition of the initial, final, and defect states, is proposed. It is shown that this mechanism is capable of explaining the observed trends in temperature dependences of the intraband relaxation rates for PbSe and CdSe colloidal nanocrystal quantum dots.
5:06PM S28.00014 Raman-Brillouin electronic density in GaAs/AlAs superlattices. NICOLAS LARGE, CEMES, Toulouse and DIPC, San Sebastian, ADNEN MLAYAH, CEMES, Toulouse, JAVIER AIZPURUA, DIPC, San Sebastian, JEAN-ROCH HUNTZINGER, GES, Montpellier, BERNARD JUSSERAND, INSIP, Paris — Raman-Brillouin scattering by acoustic phonons is an accurate experimental method to characterize vibrational states of nanostructures and understand their optical properties. Many nanoscaled systems such as quantum dots, wires, wells and membranes have been studied by the means of this technique. We present here a theoretical and experimental study of the Raman-Brillouin scattering in GaAs/AlAs superlattices. Within third order perturbation theory, we describe the Raman-Brillouin scattering process by introducing a Raman-Brillouin Electronic Density (RBED). The RBED is constructed by combining the superlattice electronic states according to their optical transition rates. This approach is useful when numerous intermediate electronic states are involved in the scattering process. It has been proven to successfully interpret the Raman-Brillouin scattering in quantum dots[1] and membranes[2]. We calculate the RBED for specific GaAs/AlAs superlattices and study the dependence of the Raman-Brillouin spectra on the GaAs/AlAs layer thickness ratio and incident photon energy. Comparison with experiments will be discussed. [1] J.R. Huntzinger et al, Phys. Rev. B 74, 115308 (2006) [2] A. Mlayah, J.R. Huntzinger and N. Large, Phys. Rev. B 75, 245303 (2007)

5:18PM S28.00015 Measured and Calculated Properties of n- and p-type PbTe-Based Materials for High-Performance Thermoelectrics1, C. VINEIS, T. HARMAN, S. CALAWA, M. WALSH, R. REEDER, W. GOODHUE, MIT Lincoln Laboratory — Recent advances in PbTe and other material systems for thermoelectric applications are based on nanostructuring, with a specific goal of substantially reducing lattice thermal conductivity while maintaining good electrical properties. Our work has focused on developing PbTe/PbSe1−xTex (x ~0.02-0.04) nanodot superlattices (NDSLs) for improved thermoelectric performance. In this presentation we will compare the electrical and thermal properties of n- and p-type NDSLs to baseline homogeneous PbTe, and also compare the electrical data to calculations performed using the Boltzmann transport equation with the relaxation time approximation. Compared to PbTe at the same carrier concentration, NDSL samples generally have reduced mobilities (~25-35%), the same Seebeck coefficients, and substantially reduced (~4-6x) lattice thermal conductivities, resulting in a large increase in ZT. Specifically, a 300-K in-plane power factor of ≥25 µW/cm-K² has been repeatedly achieved for both n- and p-NDSLs, while the cross-plane lattice thermal conductivity has been measured as ~0.35-0.4 W/m-K using various techniques. We will also present recent power generation results where 9.9 W/cm² was obtained from a 1 mm², 100-µm-thick stand-alone n-NDSL thermoelement, at a ΔT of 202 K.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S29 DMP: Focus Session: Carbon Nanotubes and Related Materials XI: Optical Spectroscopy

2:30PM S29.00001 In situ Raman Spectroscopy of Suspended Carbon Nanotubes under High Voltage Bias1, STEPHEN CRONIN, University of Southern of California — We report recent results of Raman spectroscopy taken of individual suspended single-walled carbon nanotubes exhibiting negative differential conductance (NDC) in situ under high voltage biases [1]. The transverse and longitudinal optical phonon modes (G+ and G− band) are found to respond differently to the applied voltage bias. We observe preferential downshifting of only one optical phonon mode while the other remains largely unchanged, indicating a non-equilibrium phonon population caused by the preferential electron-phonon coupling of only one optical phonon polarization. This preferential coupling is caused by the differences between the two Kohn anomalies in the TO and LO phonon branches [2]. Surprisingly, in most metallic nanotubes, the narrow G− band (TO band) is more strongly heated by electron-phonon scattering at high biases. The non-equilibrium phonon populations produced under high biases are corroborated by anti-Stokes Raman spectroscopy. We correlate the optically measured phonon population to the electrically measured resistivity using a Landauer model to determine key scattering parameters. The electron-phonon scattering mechanism revealed by these measurements and this analysis show the importance of electron-phonon scattering from absorption from the large non-equilibrium phonon population in explaining the observed negative differential conductance [3].


The authors would like to acknowledge DOE Award No. DE-FG02-07ER46376.

3:06PM S29.00002 Measurement of the absorption cross section of individual single walled carbon nanotubes. STÉPHANE BERCLAUD1, LAURENT COGNET, Centre de Physique Moléculaire Optique et Hertzienne, Université Bordeaux (France), R. BRUCE WEISMAN, Department of Chemistry, Rice University, Houston ,Texas, BRAHIM LOUNIS, Centre de Physique Moléculaire Optique et Hertzienne, Université Bordeaux (France) — We combined time–resolved and cw luminescence studies on highly luminescent individual (6,5) single walled carbon nanotubes in aqueous environments to yield the first experimental determination of the absorption cross section of individual nanotubes. Luminescence decays systematically exhibited a bi-exponential behavior with a short component (mean 45ps) accounting for most of the integrated signal, followed by a weak tail decaying on a 250 ps timescale. We obtained a mean statistical value of 1.0 10⁻¹⁷ cm² per carbon atom for nanotubes resonantly excited at their second order optical transition, a value independently obtained by photothermal absorption measurements also performed on individual (6,5) nanotubes. Precise knowledge of the absorption cross section of individual nanotubes is essential for the determination of nanotube quantum yield as well as in quantitative studies of multi-excitonic processes.

The authors would like to acknowledge DOE Award No. DE-FG02-07ER46376.

1present address: Department of Chemistry, Columbia University
3:18PM S29.00003 Length-dependent optical properties of single-walled carbon nanotubes. J. R. SIMPSON, J. A. FAGAN, B. J. BAUER, E. K. HOBBIE, A. R. HIGHT WALKER, NIST, Gaithersburg, MD 20899 — Length proves to be an important physical characteristic of single-wall carbon nanotubes (SWCNTs) strongly affecting optical absorption, photoluminescence, and resonance Raman spectroscopies. Our samples include HiPCo, CoMoCat, and arc-discharge SWCNTs dispersed in aqueous solutions by wrapping with either DNA or surfactant and exhibiting an exceptionally low degree of SWCNT bundling/clustering. Size-exclusion chromatography or density sorting ultracentrifugation collect length fractions ranging in size from approximately 50 nm to 1000 nm. The optical spectral weight specific to the SWCNT electronic states and photoluminescence peak emission intensity, compared to their underlying backgrounds, scale approximately linearly with length. All observed Raman vibrational modes exhibit a monotonic increase of scattering intensity with nanotube length. Resonance Raman of the radial breathing mode reveals a blueshift of the excitation energy for shorter nanotubes. Localization of bound excitons along the nanotube may explain the observed length-dependent optical properties.

3:30PM S29.00004 Reflectance spectra of individual single walled carbon nanotubes. HUALING ZENG — We report back scattering spectroscopic measurements on individual single walled carbon nanotubes (SWNTs). The reflectance spectra show geometry-dependent resonant peaks corresponding to optical transitions between Van Hove singularities in SWNTs’ joint density of states. All nanotubes display certain colours as their reflectance spectra demonstrate strong energy dependence. This approach was proved to be an effective tool to probe geometric structures and optical properties of individual SWNTs.

3:42PM S29.00005 Inverted spectra of SWCNT films. JOHN LEHMAN, KATHERINE HURST, LARA ROBERSON, NIST, KATHRYN NIELD, JOHN HAMLIN, MSL-New Zealand — Diffuse Reflectance for purified single wall carbon nanotube (SWCNT) films and its relation to absorptance in the wavelength range 0.6 µm to 2 µm are inverted when compared to absorptivity data in the literature. This surprising behavior has been corroborated by diffuse reflectance measurements and shows that the reflectance is a substantial part of the unique optical behavior. Typically, the absorptance is fairly assumed to be complementary to the transmittance, while the reflectivity is insignificant. Only in certain instances (see for example, Barnes, et al[1], Wang, et. al[2]), is the small reflectance explicitly accounted for. In the present work, we present diffuse reflectance and specular absorptance at normal incidence of SWCNT films.


3:54PM S29.00006 Broadband Rayleigh Scattering and Photoconductivity Spectra of Individual Semiconducting Single-Walled Carbon Nanotubes. MATTHEW SFEIR, Brookhaven National Laboratory, SAMI ROSENBLATT, YANG WU, HUGEN YAN, CHRISTOPHE VOISIN, BHUPESH CHANDRA, ROBERT C. C. CALDWELL, YUYAO SHAN, JAMES HONE, TONY F. HEINZ, Columbia University, JAMES A. MISIEWICH, Brookhaven National Laboratory — Combining a Fourier-transform measurement of photoconductivity with Rayleigh spectroscopy, we have identified the four lowest-lying optical transitions from specific, individual single-walled carbon nanotubes. In these investigations we made use of the previously reported transfer technique [1] to obtain samples with optimized arrangements both for Rayleigh (freely suspended) and photoconductivity (transistor geometry) spectroscopy. The combination of these two optical characterization techniques yields high-resolution spectra of the electronic transitions of individual nanotubes over a spectral range extending from 0.3 – 2.7 eV. We will discuss the details of the spectra that we have obtained for individual single-walled nanotubes of defined chiral index, including the observation of asymmetric lineshapes for the lowest-lying optical transition. [1] X. M. H. Huang, et al, Nano Lett. 5, 1515 (2005).

[1]This work was supported by the DOE under contract number DE- AC02-98CH10886.

4:06PM S29.00007 Optical phonon and hot carrier lifetimes in single-walled carbon nanotubes by time-resolved anti-Stokes Raman scattering. KWANGU KANG, DAVID CAHILL, TANER OZEL, MOONSUB SHIM, Frederick Seitz Materials Research Laboratory, and Department of Materials Science and Engineering, University of Illinois — The lifetimes of optical phonon and photoexcited carriers in both semiconducting and metallic single-wall carbon nanotubes are determined by time-resolved Raman scattering using a subpicosecond pump-probe method. Non-equilibrium populations of electronic and phonon excitations are observed by incoherent anti-Stokes Raman scattering from a broad continuum and the G mode, respectively. HiPCo nanotubes with E_{22} transitions and arc-discharge nanotubes with E_1 transitions dominate the spectra because of their resonance with the photon energy. To separate Raman scattering created by the probe beam from scattering created by the pump beam, we have developed a two-color pump-probe technique based on the broad bandwidth of the Ti:sapphire laser oscillator and narrow bandpass optical filters. For semiconducting tubes, the optical phonon lifetimes decrease from 1.2 ps to 0.9 ps with increasing laser fluence. The optical phonon lifetimes of metallic tubes, on the other hand, increase from 0.6 ps to 1.1 ps. The hot carrier lifetime is approximately 0.3 ps.

4:18PM S29.00008 Raman Spectroscopy of isolated Double Wall Carbon Nanotubes (DWNT). FEDERICO VILLALPANDO-PAEZ, ALFONSO REINA CECCO, Massachusetts Institute of Technology, DAISUKE SHIMAMOTO, Shinshu University, Japan, ANTONIO G. SOUZA FILHO, Universidade Federal do Ceara, Brazil, HYUNGBIN SON, Massachusetts Institute of Technology, YOONG A. KIM, ENDO MORINOBU, Shinshu University, Japan, MAURICIO TERRONES, Instituto Potosino de Investigacion Cientifica y Tecnologica, Mexico, MILDRED DESSELSHAUS, Massachusetts Institute of Technology — We have developed a method to perform Raman spectroscopy on isolated double wall carbon nanotubes (DWNT). By identifying isolated DWNTs and obtaining their Raman spectra using different laser lines, we are able to find DWNTs whose inner and outer walls are in resonance with the same laser line or with more than one laser lines ranging from 514nm to 785nm. The inner and outer walls of a DWNT can be metallic (M) or semiconducting (S) and each of the four possible configurations (M/M, M/S, S/S, S/M) has different electronic properties. The obtained Raman spectra show simplified radial breathing mode (RBM), G and G’ line shapes that allow us to study the inter layer interactions and make comparisons to previous experiments on DWNT bundles and double layer graphene.

[1]CONACYT Mexico, NSF Grant DHR04-05588
We study the transport properties of a long non-uniform quantum wire where the electron-electron interactions are treated in a tight binding formalism which includes bond-stretching, in-plane and out-of-plane bond-bending, and bond-twisting interactions. Equations of motion for the coherent phonon amplitudes are obtained in a density matrix formalism and we find that the coherent phonon amplitudes satisfy driven oscillator equations. In coherent phonon spectroscopy the coherent phonons are detected by ultrafast pump probe differential transmission measurements. We find that for uniform illumination with a 5 fs pump pulse only the q = 0 radial breathing mode and a high frequency G mode are strongly excited. We will discuss excitation strengths for different coherent phonon modes and compare to recent experiments.

1Supported by NSF DMR-0325474.

4:30PM S29.00009 Theory of coherent phonon spectroscopy in carbon nanotubes1. G. D. SANDERS, C. J. STANTON, University of Florida, Y. S. LIM, Konkuk University, K. J. YEE, J. H. KIM, Chungnam National University, E. H. HARZO, L. G. BOOSHEHR, J. KONO, Rice University — We develop a theory for the generation and detection of coherent phonons in single wall carbon nanotubes. Coherent phonons are generated in the nanotube by ultrafast laser pulses via the deformation potential electron-phonon interaction with the photogenerated carriers. The electronic states are treated in a tight binding formalism which gives a description of the states over the nanotube Brillouin zone while the nanotube phonon modes are treated in a valence force field model that includes bond-stretching, in-plane and out-of-plane bond-bending, and bond-twisting interactions. Equations of motion for the coherent phonon amplitudes are obtained in a density matrix formalism and we find that the coherent phonon amplitudes satisfy driven oscillator equations. In coherent phonon spectroscopy the coherent phonons are detected by ultrafast pump probe differential transmission measurements. We find that for uniform illumination with a 5 fs pump pulse only the q = 0 radial breathing mode and a high frequency G mode are strongly excited. We will discuss excitation strengths for different coherent phonon modes and compare to recent experiments.

1Supported by NSF DMR-0325474.

4:42PM S29.00010 Stability of carbon nanotubes to laser irradiation probed by Raman spectroscopy. ALEXANDER SOLDATOV, DAVID OLEVKI, Dept. of Physics, Lulea University of Technology, MANUEL DOSSOT, Dept. of Chemical Physics, Nancy University, EDWARD MCRRAE, Lab. of Solid State Chemistry, Nancy University — CNTs in a bundled state suffer from overheating effects — exposure to laser irradiation leads to a reversible shift of the RBM resonance window at a moderate laser fluence [1] or even to damaging of certain nanotube types at higher fluences. Here we report on our systematic study of the influence of laser irradiation on the Raman spectra of HiPCO-produced single wall CNTs. Specifically, we have examined Raman response of bundled CNTs to: i) laser power density; ii) exposure time and iii) photon energy (1.96 and 2.33 eV). Our results show that irreversible destruction of CNTs in the bundles takes place at even a moderate laser power density (~500 W/cm²). Notably, the tubes with smaller diameters are influenced first and the rate of CNT damage increases with photon energy. Finally, we determined that the threshold for the RBM spectrum profile to change at ~200 W/cm², which is apparently below the laser fluencies used typically in Raman experiments on CNT bundles. Based on these results we developed a regime of Raman data collection which was recently used to identify functionalization of different types of CNTs [2] from their Raman spectra. [1] C. Fantini, et al. Phys. Rev. Lett., 93, 147406 (2004). [2] J. Liu, et al. Carbon, 45, 885, (2007).

5:45PM S29.00011 Surface Enhanced Raman Spectroscopy (SERS) and Scanning Electron Microscopy of Individual SERS Hot Spots. RAJAY KUMAR, STEPHEN CRONIN — We measure Raman spectroscopy and scanning electron microscopy before and after depositing silver nanoparticles on carbon nanotubes. Individual SERS ‘hot spots’ are identified with respect to a lithographically defined grid and using a cross-mapping technique. Carbon nanotubes’ extremely large aspect ratio enables subsequent imaging of the nanoparticle geometry together with the SERS active molecule. The SERS enhancement factor is determined by comparing the Raman intensity of an individual nanotube before and after nanoparticle deposition. The data, published in R. Kumar et al., Appl. Phys. Lett., 91 (2007), reports SERS enhancement factors up to 134,000 and nanoparticle heating exceeding 600°C, as evidenced by the local burnout of nanotubes in SERS hot spot regions.

5:06PM S29.00012 Electrical Transport Studies of (n,n) Armchair Carbon Nanotubes. ROBERT CALDWELL, BHUPESH CHANDRA, CHRISTOPHE VOISIN, TONY F. HEINZ, JAMES HONE, Columbia University — By using Rayleigh scattering spectroscopy, a simple mechanical transfer process, and standard E-beam lithography fabrication of metallic leads, we can probe the electrical properties of individual single-walled carbon nanotubes of known chiral indices (n,m) on the substrate of our choosing. Using these techniques, we have discovered that (n,n) ‘armchair’ nanotubes consistently deviate from the predicted metallic behavior, specifically showing a gap in current – gate voltage curves. We present detailed studies of the transport behavior of these devices, including conductivity as a function of bias, length, and temperature.

5:18PM S29.00013 Supercurrent in Single Wall Carbon Nanotube Josephson Junctions. GANG LIU, YONG ZHANG, CHUNNING LAU — We investigate transport in highly transparent single-wall carbon nanotube Josephson Junctions. Gate tunable supercurrent, multiple Andreev reflections and hysteresis current-voltage characteristics are observed, corresponding to on- and off-resonance transmission of charges via the nanotube’s quantized energy levels. In the talk we will discuss the dependence of supercurrent on temperature, source-drain separation and gate voltage, and compare with various theoretical models.
3:06PM S30.00009 Microwave Kinetic Inductance Measurement of a Carbon Nanotube

Y. YIN, J. CHUDOW, J. MANO ORTEGA, A. TRUE, C. A. SCHMUTTENMAER, Dept. of Chemistry, Yale Univ., B. REULE, LPS, Université Paris-Sud, Orsay, France. — The single-wall metallic carbon nanotube is a model molecular nano-system, and has also been proposed as a candidate for future IC interconnects. For both these reasons, measurement of the kinetic inductance is desirable. This inductance arises from the kinetic energy of electrons in the four quantum channels. It is fundamental to the prediction of the Luttinger liquid theory. Direct measurements at room temperature have been reported by Intel. That measurement is very challenging due to the large resistance compared to 50 ohms, and the small inductive impedance. We propose and demonstrate a new approach which uses two on-chip transmission line resonators to transform the nanotube impedance to nearly match the 50 ohm range of the microwave network analyzer. Simulations and cryogenic measurements will be presented.

This research was supported by NSF-CHE and NSFDMR.
4:42PM S30.00013 Zone Unfolding and Approximate Bandstructure Calculations in Tight-Binding
1, TIMOTHY BOYKIN, University of Alabama-Huntsville, NEERAJ KHARCHE, Purdue University, MATHIEU LUSIER, ETH Zurich, GERHARD KLMEEK, Purdue University — Tight-binding electronic structure calculations for periodic systems are often carried out in non-primitive unit cells, or for imperfect (e.g. random-alloy) nanostructures, such as nanowires. In the first case bands exist but they are difficult to identify due to the choice of unit cell for the calculation, while in the second case bands only exist in an approximate sense. The Brillouin zone unfolding technique applied to tight-binding calculations provides a powerful tool for extracting the true primitive-cell bands from non-primitive cells. Also, it is the starting point for approximate nanowire band calculations. We discuss zone unfolding in tight-binding and its application to both perfect and imperfect systems.

1Supported by Semiconductor Research Corporation.

4:54PM S30.00013 Gate Voltage Dependent Raman Scattering from Semiconducting Carbon Nanotube FETs, JAMES TSANG, MARCUS FREITAG, VASILI PEREBEINOS, PHAEDON AVOURIS, IBM T. J. Watson Research Center — The Raman spectrum of the carbon nanotube in a carbon nanotube FET changes reversibly as a gate voltage is applied, modifying the charge density in the channel. We show that the intensity of the G-line Raman scattering from semiconducting CNTFETs can decrease with applied gate voltage. This is in addition to our previously reported shift of the G-line to higher energies with no change in spectral width as the channel charge density increases. The spectral shift has been explained by gate voltage induced changes in the electronic excitations of the carbon nanotube which interact with the G-line. The gate voltage induced G-line shift and intensity changes observed in CNTFETs are similar to the changes observed for the G-line scattering between a suspended carbon nanotube over a trench, and the same tube on the substrate, where the G-line scattering from tube on the substrate shifts to higher energies and is weaker than the G-line scattering from the suspended tube. Gate voltage or substrate induced doping effects can modify the measured intensity of the Raman spectrum of a semiconducting carbon nanotube.

5:06PM S30.00014 Directed Assembly and Electrical Characterization of Carbon Nanotube-Molecule-Metal Junctions, KANSHENG CHEN, P. XIONG, Florida State University, S.A. MCGILL, National High Magnetic Field Laboratory — Molecular-template directed assembly has been shown to be an effective method for bottom-up assembly of high-performance single-walled carbon nanotube field-effect transistors (SWNT-FETs) 1. Here, we utilize this platform to carry out a systematic study of the electron transport behavior through SWNT-molecule-metal junctions. The devices were fabricated on doped-Si/SiO2 substrates: Au source/drain electrodes were first defined by electron beam lithography. Self-assembled monolayers (SAMs) of thiol molecules with polar ends were then created on either electrode by immersing the sample in molecule solution or on one of the electrodes by dip- pen nanolithography. Finally, SWNTs were selectively self-assembled onto the electrodes by putting a drop of SWNT solution on the template. The electron transport through the molecular SAM between the SWNT(s) and the Au electrodes were characterized through gated I-V measurements. The same devices were measured before and after the desorption of the molecular SAM(by baking) to directly elucidate the role of the molecules on the electron transport. The results will be presented and discussed.


5:18PM S30.00015 Thermal Imaging of Electrically-Heated Carbon Nanotubes using Raman Spectroscopy, SCOTT HSIIE, VIKRAM DESHPANDE, California Institute of Technology, ADAM BUSHMAKER, STEVE CRONIN, University of Southern California, MARC BOCKRATH, California Institute of Technology — Suspended carbon nanotubes have been known to exhibit striking negative differential conductance under high bias voltages1. To better probe the physics underlying this phenomenon, we have recently developed techniques to measure Raman spectra simultaneously with electrical transport, resulting in the direct observation of mode selective electron-phonon coupling2. Using similar techniques, we present spatially resolved data taken from long, suspended, and electrically contacted individual carbon nanotubes. Along with electrical transport, Raman spectra are taken at several points along the spatial coordinate, creating a spatial map of the Raman-active phonon populations and the lattice temperature profile. We use a finite element simulation to corroborate our data with a Landauer model and extract numerical values for key scattering and relaxation rate parameters and thermal contact resistances. This use of Raman spectroscopy constitutes a novel non-contact technique for probing local thermal data in nanosstructures.


Wednesday, March 12, 2008 2:30PM - 5:30PM — Session S31 DMP GMAG: Focus Session: Multiferroics I: 113 and 125 Morial Convention Center 223

2:30PM S31.00001 Dynamics and Phase Transitions in Multiferroic Helimagnets, HOSHI KATSURA, Department of Applied Physics, University of Tokyo, SHIGEKI ONODA, Condensed Matter Theory Laboratory, RIKEN, JUNG HOOON HAN, Department of Physics and Institute for Basic Science Research, Sungkyunkwan University, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo, CERC, CREST — The strong coupling between magnetism and ferroelectricity in multiferroics has recently been attracting much attention due to the fundamental physics involved and promising applications. The representative materials are helical magnets RMnO3 (R =Gd,Tb,Dy) and they have been extensively studied experimentally. We theoretically studied the dynamics and phase transitions in cycloidal helical magnets showing the multiferroic behavior. Our approach reproduces several novel features such as the anomalous dielectric response revealed by recent experiments on RMnO3 [1,2]. We also study the nature of the phase transition from collinear to helical spin structure. [1]N. Kida, Y. Ikebe, Y. Takahashi, J. P. He, Y. Kaneo, Y. Yamasaki, R. Shimano, T. Arima, and Y. Tokura, [arXiv:0711.2733]. [2]A. Pimenov, A. Loidl, A. A. Mukhin, V. D. Travkin, V. Yu. Ivanov, and A. M. Balbashov, [arXiv:0707.3614].

2:42PM S31.00002 Novel coupling of Tb- and Mn-magnetic orders in multiferroic TbMnO3, D.N. ARGIYROU, O. PROKHENKO, R. FEYERHERM, Hahn-Meitner-Institut, Glienicker Str. 100, Berlin D-14109, Germany, M. MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, Netherlands, N. ALIOUANE, E. DUDZIK, A.U.B. WOLTER, A. MALJUK, Hahn-Meitner-Institut, Glienicker Str. 100, D-14109 Berlin, Germany — We report on diffraction measurements on multiferroic TbMnO3 which demonstrate that the Tb- and Mn-magnetic orders are coupled below the ferroelectric transition TF,E =28 K. For T < TF,E the magnetic propagations vectors (τ) for Tb and Mn are locked so that τTb=τMn, while below TFB=E =7 K we find that τTb and τMn lock-in to rational values of 3/7b* and 2/7b* respectively, and hold the relationship 3τTb+τMn = 1. We explain this novel matching of wave vectors within the frustrated ANNNI model coupled to a periodic external field produced by the Mn-spin order. The τTb=τMn behavior is recovered while the τTb=3/7 regime is stabilized by an optimal Tb spin-density wave ordering with 6 domain walls, superimposed on the τMn=2/7 Mn-ordering.

Wednesday, March 12, 2008 2:30PM - 5:30PM — Session S31 DMP GMAG: Focus Session: Multiferroics I: 113 and 125 Morial Convention Center 223
Electric polarization reversal in multiferroic TbMnO$_3$ with rotating magnetic field direction. NOBUYUKI ABE, SHINTARO OHTANI, Department of Physics, Tohoku University, KOUJI TANIGUCHI, TAKA-HISA ARIMA, IMRAM, Tohoku University, TAISHI TAKENOBU, YOSHIHIRO IWASA, IMR, Tohoku University — Recent extensive studies of magneto-electric multiferroics have revealed that the magnitude and direction of electric polarization can be considerably modified by the application of a magnetic field. TbMnO$_3$ is a prototypical multiferroic which shows the electric polarization flop from $P // c$ to $P // a$ by the application of magnetic field along the $b$ or $a$ axis. We have found that the direction of the magnetic-field induced polarization along the $a$-axis ($P_a$) is memorized even in the zero field where $P_a$ is absent. The polarization direction can be reversed by rotating the magnetic field direction in the ab plane. For the memory application of the multiferroic material, such a bistability in zero field and a switching between the bistable states with some nonoverlapping stimulus are essential.

Spiral magnetic order in the ferroelectric phase of Gd$_{0.7}$Tb$_{0.3}$MnO$_3$. YUCHI YAMASAKI, Y. TOKURA, K. SASAI, M. MATSUURA, K. HIROTA, University of Tokyo, 6-7-1 Hongo, Bunkyo-ku, Tokyo 113-0033 Japan, KOUJI TANIGUCHI, TAKA-HISA ARIMA, Y. NODA, Tohoku University — Perovskite manganite Gd$_{0.7}$Tb$_{0.3}$MnO$_3$ possesses a ferroelectric phase with an electric polarization along the $a$ axis ($P||a$) in zero magnetic field, while RSmMnO$_3$ ($R$=Tb and Dy) undergo ferroelectric transitions with $P$ along the $c$ axis ($P||c$). The $P||a$ phase emerges upon the incommensurate to commensurate transition of the lattice modulation in a similar way of the magnetic field induced $P||a$ phase of TbMnO$_3$. The polarized neutron diffraction and the magnetic structure analysis of the $^{155}$Gd$_{3+}$-enriched single crystal of Gd$_{0.7}$Tb$_{0.3}$MnO$_3$ were performed to uncover the coupling between the magnetic order and the ferroelectric polarization $P||a$ on a microscopic level. We found that the ferroelectric transition occurs concomitantly with the collinear to spiral spin transformation and the spin helicity can be controlled by the electric field applied on cooling. Namely, the ferroelectric polarization in the $P||a$ phase can be explained by the spin current model as well as the $P||c$ phases known for TbMnO$_3$.

Reentrant electromagnons in multiferroic Eu$_{0.75}$Y$_{0.25}$MnO$_3$ in the H-T phase diagram. ROLANDO VALDES AGUILAR, A.B. SUSHKOV, H.D. DREW, MRSEC, Department of Physics, University of Maryland, College Park, MD 20742, J.Y. CHOI, C. ZHANG, S-W. CHEONG, Rutgers University, Piscataway, NJ 08854 — The electromagnon spectra of Eu$_{0.75}$Y$_{0.25}$MnO$_3$ has been measured as a function of magnetic field $H$ || c up to 8 T and temperature between 5 and 300 K. Three magnetic induced electric dipole features reported earlier are observed to weaken simultaneously but not shift for increasing field. These electromagnons features all show reentrant behavior as a function of temperature for $H > 6$ T and with the anomalies in the static dielectric constant, confirming their electromagnon origin. While the magnetic structure of Eu$_{0.75}$Y$_{0.25}$MnO$_3$ is unknown, it is assumed that it is a cycloidal magnet where the spins lie in the crystallographic a-b plane, based on the behavior of the magnetic susceptibility and the direction of static polarization $P$. Therefore, it appears that the electromagnon selection rule, $|\epsilon\alpha\alpha|$, in all the multiferroic RSmMnO$_3$ magnetics is independent of the spin plane and polarization direction. We will compare the phase diagrams of Eu$_{0.75}$Y$_{0.25}$MnO$_3$ and TbMnO$_3$ where similar anomalies are observed.

Reentrant electromagnons in multiferroic Eu$_{0.75}$Y$_{0.25}$MnO$_3$. DIYAR TALBAYEV, ANTOINETTE J. TAYLOR, Los Alamos National Laboratory, RICHARD D. AVERITT, Boston University, CHENGLIN ZHANG, SANG-WOOK CHEONG, Rutgers University — Dynamical studies of multiferroic materials help unravel the fundamental interactions between various degrees of freedom and answer technological questions such as achievable switching speeds in multiferroic-based memory elements. We report the results of the ultrafast pump-probe reflectance study of multiferroic Eu$_{0.75}$Y$_{0.25}$MnO$_3$. The material undergoes antiferromagnetic ordering and, upon further cooling, ferroelectric ordering that strongly couples to the material’s magnetic state. We measured the relaxation time of the pump-probe reflectance in this compound using 800-nm pump and probe pulses. The temperature dependence of the relaxation time follows that of the low-energy spectral weight that includes phonons and electro-active magnons [1]. This suggests a strong coupling between electronic (1.55 eV) and low-energy electro-active excitations in Eu$_{0.75}$Y$_{0.25}$MnO$_3$ that can be tuned by magnetic field. The relaxation time increases upon the application of magnetic field along the crystal’s c-axis in the ferroelectric phase, but exhibits no change in the paraelectric phase. Our results indicate the importance of multiple energy scales (electronic, lattice, and magnetic) for the multiferroicity of Eu$_{0.75}$Y$_{0.25}$MnO$_3$. 1. R. Valdes Aguilar et al, Phys. Rev. B 76, 060404(R) (2007)

Theory of terahertz absorption spectra due to two-magnon processes in cycloidal spin magnets. SHIN MIYAHARA, Multiferroics Project (MF), ERATO, Japan Science and Technology Agency (JST), NOBUO FURUKAWA, Aoyama Gakuin University — Perovskite manganites $RMnO_3$ have an attraction both experimentally and theoretically after the discovery of the ferroelectric polarization and its flop by external magnetic field. Recently the measurements by the terahertz time-domain spectroscopy have been investigated with the several sets of light polarization, and novel magnon states induced by the electric field are observed. Such a spin excitation is called an electromagnon. However, the origin of the electric-dipole active absorption is not clarified yet. We calculated the absorption of light due to the electric dipole transitions associated with two-magnon excitations in cycloidal spin magnets. The theory is applied to the ferroelectric magnets $RMnO_3$, and absorption peaks in terahertz time domain spectroscopy, which correspond to electromagnons, are interpreted with reasonable parameter sets.

Resonant magnetic scattering of multiferroic HoMnO$_3$ in an applied electric field. S. NANDI, A. KREYSSIG, L. TAN, J.W. KIM, J.Q. YAN, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State Univ., J.C. LANG, D. HASKEL, Advanced Photon Source, Argonne National Laboratory, R.J. MCQUEENEY, A.I. GOLDMAN, Ames Laboratory and Dept. of Physics and Astronomy, Iowa State Univ. — The multiferroic material HoMnO$_3$ displays electrical polarization $P_c = 5.6 \mu$C cm$^{-2}$ along the hexagonal c axis below the Curie temperature $T_C = 875$ K and antiferromagnetic Mn$^{3+}$ ordering at the Néel temperature, $T_N = 75$ K. The recently reported ferromagnetic response of Ho$^{3+}$ by an applied electric field opens up the possibility of electric field controlled magnetic data storage. However, both the role of Ho$^{3+}$ in magnetism and details of the magnetic structure of Ho$^{3+}$ have been topics of significant debate. Using element specific x-ray resonant magnetic scattering and x-ray magnetic circular dichroism, we have focused on resolving this controversy. Both quadrupole and dipole Ho $L_{111}$ resonances were observed below 40 K. In zero field, Ho$^{3+}$ orders antiferromagnetically with moments along the c direction below 40 K and undergoes a transition to a different magnetic order below 4.5 K. The role of Ho$^{3+}$ upon the application of an external electric field in the temperature range 1.7-80 K will be discussed. – The support by U.S. DOE (DE-AC02-07CH11358 and DE-AC02-06CH11357) is acknowledged.
measurements suggest that Dy plays an active role in enhancing the ferroelectric polarization in multiferroic DyMnO$_3$.

Hahn-Meitner-Institut, Glienicker Str. 100, Berlin D-14109, Germany — Neutron powder diffraction and single crystal x-ray resonant magnetic scattering evolution of an incommensurate ordering of Dy moments with the same periodicity as the Mn spiral ordering. It closely tracks the evolution of the ferroelectric polarization. Below $T_{N}^{Dy}$, where Dy spins order commensurately, the polarization decreases to values similar for those of TbMnO$_3$. The higher $P_s$ found just above $T_{N}^{Dy}$ arises from the contribution of Dy-spins so as to effectively increase the amplitude of the Mn spin-spiral.

1 Corresponding Author

4:18PM S31.00010 Electrically driven spin excitation in a ferroelectric magnet DyMnO$_3$. N. KIDA, Multiferros Project, ERATO, JST, Y. IKEBE, Univ. Tokyo, Y. TAKAHASHI, J.P. HE, Y. KANEKO, Multiferros Project, ERATO, JST, Y. YAMASHI, Univ. Tokyo, R. SHIMANO, Multiferros Project, ERATO, JST and Univ. Tokyo, T. ARIMA, Tohoku Univ., N. NAGAOUSA, Univ. Tokyo and RIKEN, Y. TOKURA, ERATO-JST, Univ. Tokyo, and RIKEN — In multiferroic manganites, there have been recent experimental and theoretical arguments on the possibility of the presence of the low-lying spin excitation, called electromagnon, where the spin excitation electrically becomes active [1]. Here we report on a complete set of low-energy (1–10 meV) electrodynamics of spin excitations for a multiferroic DyMnO$_3$ with variations of the light polarization in a variety of phases tuned by both temperature (5–250 K) and magnetic field (0–70 kOe) [2]. We identify the pronounced absorption continuum (1–8 meV) with a peak feature around 2 meV, which is electric-dipole active only for the light E-vector along the a-axis. This absorption band grows in intensity with lowering temperature from the spin-collinear paraelectric phase above the ferroelectric transition, but irrespectively of the direction of the bc or ab spiral spin plane. The possible origin of this electric-dipole active band is argued in terms of the gigantic fluctuations of spins and spin-current. [1] A. Pimenov et al., Nat. Phys. 2, 97 (2006). [2] N. Kida et al., arXiv:0711.2733

4:30PM S31.00011 Spin structures of magnetic phases in YMn$_2$O$_5$. J.-H. KIM, S.-H. LEE, University of Virginia, S. WAKIMOTO, M. MATSUDA, JAE, H. KIMURA, Y. NODA, Tohoku University, S. JUERG, PSI, M. KENZELMANN, ETH/PSI, C.F. MAJKRZAK, NIST, S.-I. PARK, KAERI, S. PARK, S.W. CHEONG, Rutgers University — A magnetic ferroelectric material, YMn$_2$O$_5$, undergoes several magnetic phase transitions at low temperatures and develops spontaneous electric polarization along the b-axis in a commensurate magnetic phase with a characteristic wave vector of (0.5,0.0,0.25). We have determined the commensurate spin structure by performing four circle neutron diffraction (FCD) and three-dimensional polarization analysis (CRYOPAD) on a single crystal of YMn$_2$O$_5$. In the spin structure, Mn$_4^+$ moments form a transverse (cycloidal) spiral structure along the c-axis that can induce the spontaneous electric polarization along the b-axis.

4:42PM S31.00012 Magnetic domains in multiferroic YMn$_2$O$_5$ probed by Spherical Neutron Polarimetry under electric field. CARLO VECCHINI, LAURENT CHAPON, PAOLO RADAELLI, AZIZ DAOUD-ALADINE, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, UK11 0QX, UK, JANE BROWN, TAPAN CHATTERJI, Institut Laue-Langevin, 6, rue Jules Horowitz, BP156-38042 Grenoble Cedex 9 - France, SOONYONG PARK, SANG-WOOK CHEONG, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Precise determination of the magnetic structures in multiferromagnetic materials, YMn$_2$O$_5$, can be obtained by single crystal neutron diffraction. The analysis shows the presence of zig-zag antiferromagnetic chains in the ab-plane. An additional weak magnetic component parallel to the c-axis was detected which is modulated in phase quadrature with the a-b components. The nature and population of the coexisting antiferromagnetic domains in YMn$_2$O$_5$ have been determined by Spherical Neutron Polarimetry under an external electric field. We have proved that reversing the electrical field results in the inversion of the population of two types of antiferromagnetic domains, with opposite in-plane spin components. This analysis strongly supports theories in which the coupling of the magnetic configuration to the ferroelectric polarization is due to magnetic exchange striction and likely not related to the small cycloidal modulation in the bc-plane.

5:06PM S31.00013 Electromagnon H-T phase diagram of multiferroic TbMn$_2$O$_5$. DENNIS DREW, ANDREI SUSHKOV, ROLANDO VALDES AGUILAR, Department of Physics, University of Maryland, College Park MD, SOONYONG PARK, SANG-WOOK CHEONG, Rutgers University, Piscataway, New Jersey 08854, USA — We report the results of infrared (5–250 cm$^{-1}$) transmission study of multiferroic TbMn$_2$O$_5$ as a function of temperature (3–300 K) and H on magnetic fields up to 8 T. Our major observation is that the main electromagnon feature softens without splitting with increasing field at T = 5 K. This observation is in contrast with the gradual suppression of electromagnons without shifting by magnetic field in RmnO$_3$ compounds. Also, it is in agreement with the theoretical prediction of Fang and Hu [2] for this system. In this talk, we will also discuss other features of the magnetic field dependence of the low energy electromagnon excitations in multiferroic TbMn$_2$O$_5$.

1 Work supported in part by NSF-MRSEC under grant DMR-0520471
2 C. Fang and J. Hu, condmat/0703487

5:50PM S31.00014 Far Infrared Anomalies in Orthorhombic Multiferroics (Bi,Pr)Mn$_2$O$_5$. N.E. MASSA, LANIS EFO-CEQUINOR, UNLP, CP 962, 1900, La Plata, Argentina, D. DE SOUSA MENESES, P. ECHEGUT, CNRS- CRMHT-F45071, Orleans, France, M.J. MARTINE-LOPE, J.A. ALONSO, CSIC-ICMM-Cantoblanca, E28049 Madrid, Spain — We report on far infrared reflectivity between 4 K and 300 K of polycrystalline BiMn$_2$O$_5$ and PrMn$_2$O$_5$ known to sustain orbital, lattice, charge, and spin interactions. After conventional temperature mode stiffening band profiles undergo a relative intensity raise with maximum in the interval ~40K to ~30 K (magnetic ordering temperature, T_N, and the onset of ferroelectricity, T_{C2}) indicative of a general electric polarization. We do not observe on cooling, in agreement with our high resolution neutron diffraction patterns, new phonon patterns which might be associated to structural changes. Below 30 K there is a weak reflectivity attenuation at about the temperature in which the spin glass sets in. In contrast, in PrMn$_2$O$_5$, we found a Drude shaped overdamped band centered at zero frequency that, active at all temperatures, develops substructure below 15 K. We associate this feature to collective modes responsible for ferroelectricity of magnetic origin ascribed to coupling spins with electronic polarization without atomic displacement. In overall, our spectra suggest a qualitative agreement with magnetoferroelectricity originating in spin dislocation and commensuration.

5:18PM S31.00015 Magnetic X-ray scattering in multiferroic HoMn2O5. LAURENT CHAPON, ISIS, Rutherford Appleton Laboratory, GUILLEAUME BEUTIER, ALESSANDRO BOMBARDI, Diamond Light Source, Rutherford Appleton Laboratory, CARLO VECCHINI, PAOLO RADAELLI, ISIS Facility, Rutherford Appleton Laboratory, S. PARK, SANG-WOOK CHEONG, Rutgers University — The commensurate magnetic phase of multiferroic HoMn2O5 has been identified by magnetic scattering off resonance and at the L3 edge of Holmium. The magnetic ordering of the Manganese ions below 40 K induces a magnetic order of Ho. Due to the element selectivity of the technique we were able to extract the temperature dependence of the Ho ordering up to temperature very close to TN. Azimuthal scans confirm the recent model of the magnetic structure determined from single neutron diffraction data, for both the Manganese and Holmium ions. The d-f coupling is discussed in the light of these results.
2:30PM S32.00001 Bound states in electronic transport through Fe/MgO tunnel junctions. IVAN RUNGER, NADJIB BAADJI, STEFANO SANVITO, School of Physics and CRANN, Trinity College, Dublin 2, Ireland — Using the ab initio code Smeagol we calculate the electronic transport properties of Fe/MgO/Fe(100) tunnel junctions for applied bias up to 2 Volt. The correct bias-dependent occupation of the interface states (IS) in the Fe/MgO junction is crucial to obtain a physically meaningful potential drop. The coupling of the IS to the Fe electrodes varies strongly for different k-points, and bound states are found along the high symmetry lines and at those k-points where there are no open channels in the Fe leads. A general method for setting the occupation of both weakly-coupled and bound states, based on the notion of a local Fermi energy and a finite relaxation time, is presented. For parallel alignment of the Fe leads the current through the IS is quenched above 20 mV, whereas for the anti-parallel alignment the current flows mainly through IS up to about 0.4 V. In this bias range the TMR shows a pronounced bias dependence, at higher voltages it decays smoothly. If the transmission through the IS is suppressed, for example by adding a finite imaginary part to the energy, the TMR decays monotonically with bias even at low voltage. Finally we show that oxygen vacancies inside the MgO barrier quench the TMR if they are within the first few layers from the interface, and that a similar reduction is achieved by partially oxidizing the Fe interface layer.

2:42PM S32.00002 Fabrication and characterization of fully epitaxial Fe/MgO/Fe magnetic tunnel junctions on Si(100) and the influence of MgO buffer layer1. G. X. MIAO, M. V. VEENHUIZEN, MIT, M. MUNZENBERG, Universitat Gottingen, J. S. MOODERA, MIT — Spin injection into Si can integrate the spin degree of freedom into future semiconductor technology. Coherent tunneling through epitaxial MgO barrier due to symmetry filtering is expected to yield large spin polarization [1]. Here we report the MBE growth of fully epitaxial Fe/MgO/Fe MTJ stacks on top of Si(100) with epitaxial MgO buffer layer giving rise to a large TMR. Due to the large lattice mismatch between Si and MgO (~9.6%), the crystalline structure of MgO is critically dependent on its thickness, and the influence is subsequently passed on to the MTJ structure. We observe a systematic change of TMR with the buffer layer thickness, which we attribute to the effect of dislocations. Coherent growth of MTJ on top of Si is a significant step toward spin injection into Si [2]. 1. W. H. Butler et al., Phys. Rev. B, 63, 054416 (2001).

2:54PM S32.00003 Temperature and Angular Dependences of Dynamic Spin-Polarized Resonant Tunneling1. CASEY W. MILLER, University of South Florida, Tampa FL 33620, USA, JOHAN ÅKERMANN, YAN ZHOU, Royal Institute of Technology, Electrum 229, 164 40 Kista, Sweden, RENU DAVE, JON SLAUGHTER, Technology Solutions Organization, Freescale Semiconductor, Inc., Chandler AZ 85224, USA, IVAN K. SCHULLER, UC San Diego, La Jolla CA 92039, USA — The bias dependence of tunneling magnetoresistance oscillations due to dynamic resonant tunneling in CoFeB/MgO/NiFe magnetic tunnel junctions was studied as functions of temperature and the relative magnetization angle of the two magnetic layers. The effect of temperature is consistent with thermal smearing, while that of the relative magnetic orientation was typical of a spin valve. A model of tunneling between spin-split free electron bands using the exact solution of the Schrödinger equation for a trapezoidal tunnel barrier agrees with experiment.

3:06PM S32.00004 Transport and spin transfer torques in Fe/MgO/Fe tunnel barriers. CHRISTIAN HEILIGER, CNST, NIST, Gaithersburg, MD / NanoCenter, UMD, College Park, MD — The prediction of very high tunneling magnetoresistance (TMR) ratios in crystalline Fe/MgO/Fe [1,2] tunnel junctions has been verified by a number of experiments [3,4]. The high TMR can be understood in terms of the electronic structure of the system. In MgO the Δ±1 states at the Brillouin zone center decay the most slowly and dominate the tunnelling current. For coherent interfaces, which are affected more strongly by the small lattice mismatch between Fe and MgO, these Δ±1 states at the Brillouin zone center are half-metallic in the Fe layers. The dominance of the Δ±1 states and their half-metallicity cause the high tunneling magnetoresistance measured in Fe/MgO/Fe tunnel junctions [5]. For the spin transfer torque, we calculate the linear response for small currents and voltages. Our calculations show that the half-metallicity of the Fe Δ±1 states leads to a strong localization of the spin transfer torque to the interface. As a result, the linear current dependence of the torque in the plane of the two magnetizations is independent of the free layer thickness for more than three monolayers of Fe. For perfect samples we also find a linear current dependence of the out-of-plane component. However, this linear piece oscillates rapidly with thickness and averages to zero in the presence of structural imperfections like thickness fluctuation, in agreement with experiment [6].

This work is supported by NSF grant and KIST-MIT funds.

3:09PM S32.00005 Tunneling Magnetoresistance in MgO based double-barrier Magnetic Tunnel Junctions1. WEIGANG WANG, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, CHAOYING NI, Department of Materials Science and Engineering, University of Delaware, Newark, Delaware 19716, Q. WEN, H.W. ZHANG, University of Electronic Science and Technology of China, Chengdu, 610054, China, TAKAHIRO MORIYAMA, JOHN XIAO, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716 — Double-barrier magnetic tunnel junctions (DMTJs) have attracted much attention due to their fertile physics and promising applications in spintronics devices. Here we report the fabrication and characterization of DMTJs of Si/ SiO2/Ta 7/Ru 20/Ta 7/CoFe 2/IrMn 15/CoFe 2/Ru 1.7/CoFeB 3/MgO 2/CoFeB 3/MgO 2/CoFeB 3/Ru 1.7/CoFe 2/IrMn 15/Ta 8/Ru 10, where the numbers are layer thickness in nanometers. Single barrier MTJs with similar structure were also fabricated. While the DMTJs exhibit the tunnel magnetoresistance (TMR) of 185 % at room temperature, which is the highest value in DMTJs reported to date, the corresponding single barrier MTJ shows 300% TMR. The reduction of TMR in DMTJs is understood in terms of sequential tunneling through two junctions in series. The effects of annealing temperature and bias voltage on the TMR of DMTJs will also be discussed.

This work is supported by NSF DMR Grant No. 0405136.
3:54PM S32.00006 Influence of spin accumulation on superconducting properties of aluminum layers in magnetic double tunnel junction devices. SEE-HUN YANG, HYUNSOO YANG, IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA, SABURU TAKAHASHI, SADAMICHI MAEKAWA, [1] Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, STUART PARKIN, IBM Almaden Research Center, 650 Harry Road, San Jose, California 95120, USA, IBM ALMADEN RESEARCH CENTER TEAM, TOHOKU UNIVERSITY COLLABORATION — We discuss the influence of spin accumulation on the superconducting (SC) properties of thin aluminum layers in crystalline MgO barrier based magnetic double tunnel junction devices composed of ferromagnet-insulator-superconductor-insulator-ferromagnet (FISIF) structures. Below the Al SC transition temperature, when the magnetization directions of the two outer CoFe ferromagnetic layers are antiparallel, the SC energy gap of the Al layer is suppressed, as compared to the case for parallel orientation of these same layers. This is consistent with theoretical models in which spin polarized quasi-particles are accumulated in the SC layer. The accumulated spin depends on the rate at which spin polarized current is injected and leaves and, most importantly, on the spin relaxation rate of the injected quasi-particles. We discuss the dependence of the spin accumulation on the spin-injection rate, which can be varied at a fixed voltage, by varying the MgO barrier thickness.

4:06PM S32.00007 Enhanced tunneling spin polarization by amorphizing usually crystalline CoFe alloys without any glass forming additives. LI GAO[1], XIN JIANG, SEE-HUN YANG, PHILIP M. RICE, STUART S.P. PARKIN, IBM RESEARCH DIVISION, ALMADEN RESEARCH CENTER, SAN JOSE, CA 95120, USA COLLABORATION — Ferromagnetic alloys of Co and Fe are particularly useful electrodes in magnetic tunnel junctions because they exhibit high spin polarization and high Curie temperatures as well as high thermal stability. These alloys are crystalline but they can be made amorphous by adding suitable glass-forming elements such as Boron. Here we show that films of pure CoFe alloys can be made amorphous, without the need of any additives, by sandwiching them between two amorphous layers, a tunnel barrier formed from amorphous Al2O3 and an amorphous overlay layer. The films are amorphous when thinner than ~25 Å but are crystalline for thicker layers. We find that both the tunneling magnetoresistance and the tunneling spin polarization (measured using superconducting tunneling spectroscopy in related junctions) are significantly enhanced when the alloy is amorphous. However, by heating the alloy above its glass crystallization temperature the enhancement is observed to vanish. Possible reasons for this behavior are discussed.

1 Department of Applied Physics, Stanford University, Stanford, CA 94305, USA

4:18PM S32.00008 Tunneling Anisotropic Magnetoresistance in Co/AIOx/Au Tunnel Junctions[1]. RUISHENG LIU, Halmstad University and Lund University, Sweden, LUKASZ MICHALAK, CARLO CANALI, Kalmar University, Sweden, LARS SAMUELSON, Lund University, Sweden, HANAN PETTERSSON, Halmstad University, Sweden — We observe spin-valve-like effects in nano-sized thermally evaporated Co/AIOx/Au tunnel junctions. The tunneling magnetoresistance is anisotropic and depends on the relative orientation of the magnetization direction of the Co electrode with respect to the current direction. We attribute this effect to a two-step magnetization reversal and an anisotropic density of states resulting from spin-orbit interaction. The results of this study points to future applications of novel spintronics devices involving only one ferromagnetic layer.

1 The authors acknowledge financial support from Halmstad University, Kalmar University, the Swedish National Board for Industrial and Technological Development, the Office of Naval Research, KAWF and SSF.

4:30PM S32.00009 Transport Studies of reduced RA product MTJs produced by highly charged ion irradiation. JOSHUA POMEROY, HOLGER GRUBE, National Institute of Standards and Technology — As is commonly known, magnetic tunnel junctions (MTJs) are used for hard drive read heads and are actively being developed for MRAM. In both of these cases, the resistance-area (RA) product is a critical parameter for device speed and bandwidth as well as total power dissipation (particularly for current driven devices). We present transport studies of MTJs whose barrier oxide has been partially reduced by highly charged ions (HCIs). The bias, temperature, and applied field dependence of these devices will be discussed. Beyond magnetic memory applications, HCI modified MTJs provide a compelling new route for preparing order THz spin torque oscillators.

4:42PM S32.00010 Large voltage from spin pumping in magnetic tunnel junctions. ZHIFANG LIN, Fudan University, SIU TAT CHUI, University of Delaware — We studied the response of a ferromagnet-insulator-normal metal tunnel structure under an external oscillating radio frequency (R.F.) magnetic field. The D.C. voltage across the junction is calculated and is found not to decrease despite the high resistance of the junction; instead, it is of the order of μV to 100μV, much larger than the experimentally observed value (100 nano-V) in the "strong coupled" ohmic ferromagnet-normal metal bilayers. This is consistent with recent theoretical results in tunnel structures, where the voltage is larger than μV.


5:06PM S32.00012 Space-Charge Induced Pauli Blockade Effect in Tunnel Junctions with Half-Metallic Electrodes[1]. A. P. LI, T.-H. KIM, X.-G. ZHANG, Oak Ridge National Laboratory, J. F. FENG, X. F. HAN, Chinese Academy of Science, Y. WANG, J. ZOU, The University of Queensland, D. B. YU, Grien Advanced Materials Co., Ltd., H. YAN, Beijing University of Technology — A space-charge induced Pauli spin blockade effect has been observed in the magnetic tunnel junction consisting of La0.95Sr0.05MnO3 (LSMO) and SrTiO3 barrier at temperatures up to 100 K. The blockade voltage under zero magnetic field provides a direct measurement of the energy gap between the Fermi energy and the top of the minority spin valence band of the LSMO. Outside the spin blockade regime, the low temperature conductance oscillates with the bias voltage as the trap centers are charged by electrons. The spin blockade can be lifted when the trap levels are thermally activated or when a large magnetic field lowers the LSMO minority spin mobility edge to below the Fermi energy. A very large magnetoresistance up to 10000% is observed and is correlated to the blockade effect. *Email: apli@ornl.gov

1 A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.
5:18PM S32.00013 First-principles theory of nonequilibrium vertex correction: disordered magnetic tunneling junction. YOUGI KE, KE XIA, HONG GUO, McGill University, HONG GUO TEAM, KE XIA TEAM — The Kubis-Nash Green's Function (NEGF) formalism has been developed within DFT to calculate the electronic structure of disordered systems. The conditionally averaged NEGF is evaluated by the vertex correction. The disordered Fe/Va/Fe tunneling junctions are investigated with present first principle method, the vertex correction shows important role in both the electronic structure and transport calculations. The bias dependence of Tunneling Magnetoresistance (TMR) in the disordered Junctions and the disordered dependence of TMR at a finite Bias were illustrated.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S33 GMAG FIAP DMP: Focus Session: Mostly III-V Semiconductors

2:30PM S33.00001 Strain-induced Fermi contour anisotropy of GaAs (311)A 2D holes. JAVAD SHABANI, MANSOUR SHAYEGAN, Department of Electrical Engineering, Princeton University, ROLAND WINKLER, Department of Physics, Northern Illinois University — There is considerable current interest in electronic properties of two-dimensional (2D) carriers whose energy bands are split at finite values of in-plane wave vector, thanks to the spin-orbit interaction and the lack of inversion symmetry. We report experimental and theoretical results revealing that the spin-subband Fermi contours of the heavy and light heavy-holes (HHh and HHH) can be tuned in high mobility GaAs (311)A 2D hole systems via the application of symmetry-breaking in-plane strain. Our calculations show that the HHH spin-subband Fermi contour is circular but the HHh spin-subband Fermi contour is distorted. Experimentally, we prove the Fermi contour anisotropy by measuring the magneto-resistance commensurability peaks induced by square arrays of antidots. When the spin splitting is sufficiently large, the magneto-resistance trace exhibits two peaks, providing clear evidence for spin-resolved ballistic transport. The experimental results are in good agreement with the calculations, and confirm that the majority spin-subband (HHH) has a severely distorted Fermi contour whose anisotropy can be tuned with strain while Fermi contour of the minority spin-subband (HHH) remains nearly isotropic.

2:42PM S33.00002 Strain-induced spin splittings in III-V and II-VI semiconductors. B.J. MOEHLMANN, MICHAEL E. FLATTÉ, OSTC and Department of Physics and Astronomy, University of Iowa — We have calculated the strain-induced spin splittings in III-V and II-VI semiconductors using a fourteen-band basis for a strain-dependent k - p Hamiltonian. Using deformation potentials from pseudopotential calculations we find quantitative agreement with the precessional rates observed in [1]. For GaAs, the contribution of upper-conduction-band deformation potentials to the strain-induced spin splitting is not negligible. The ratio of the strain-induced spin precession frequency to the drift velocity is similar for GaAs and InAs, but is an order of magnitude larger for GaSb and InSb. For ZnSe it is a factor of 2 smaller than GaAs. This work was supported by an ONR MURI. [1] Kato et al., Nature 427, 50 (2004).

2:54PM S33.00003 Electric field dependent g tensor modulation for a hydrogenic Si donor in bulk GaAs1. AMRIT DE, CRAIG E. PRYOR, MICHAEL E. FLATTÉ, Department of Physics and Astronomy and Optical Science and Technology Center, University of Iowa — We present calculations demonstrating the feasibility of electrical manipulation of a donor bound electron spin using g tensor modulation resonance. We calculate the electron g factor as a function of applied electric field, and show that dxy/dE is largest when the applied magnetic and electric fields are parallel. Unlike quantum dots, the donor’s g factor is highly nonlinear as a function of the applied magnetic field, and the anisotropy of the g tensor also has a strong magnetic field dependence. The calculations are for a Si impurity in GaAs, and are done using real-space 8-band k-p theory in the envelope approximation.

3:06PM S33.00004 Gilbert Damping in (Ga, Mn) As , ION GARATE, ALLAN MACDONALD, University of Texas at Austin — We examine Gilbert damping in (Ga,Mn)As by using a p-d mean-field theory model for the ferromagnetic ground state and a four-band spherical model for the host semiconductor band structure. Within this model it is possible to calculate impurity vertex- corrections to the long-wavelength spin-spin response functions to all orders. Because of spin-orbit coupling in the band structure, beyond leading order vertex corrections make significant contribution to the damping. We comment on the non-monotonic dependence of damping on impurity strength.

3:18PM S33.00005 Magnetic patterning of GaMnAs layers by hydrogen passivation. L. THEVENARD, A. LEMAITRE, G. FAINI, Lab. Photonique et Nanostructures, N. VERNIER, J. FERRE, Lab. Physique des Solides, S. FUSIL, UMR CNRS Thales — In order to study the magnetic switching behavior of diluted magnetic semiconductor (DMS) microstructures, we have patterned thin layers of (Ga,Mn)As by an original method. We have used local hydrogen passivation to locally suppress the carrier-mediated ferromagnetic phase. This purely diffusive process maintains the continuity of the film and smooths border effects. Two types of structures were examined by Kerr microscopy, and their magnetic behavior compared to that of structures made by dry etching1. On hydrogenated arrays of micron-sized magnetic dots, the switching fields were closer to the continuous film coercivity, and with a smaller dispersion. On micron-wide magnetic stripes, current-induced domain wall (DW) propagation was observed with typical currents as low as j = 4×107 A·cm⁻², a result of the low edge roughness induced by the patterning, and the low density of magnetic atoms. Local hydrogen passivation therefore appears as a viable route towards lower injection currents in DMS spintronics devices based on DW manipulation. 1 L. Thevenard et al., Appl. Phys. Lett. 91, 142511 (2007)

3:30PM S33.00006 Infrared longitudinal and Hall conductivities in Ga1−xMnx As films. HEORGHIE AGBAS, M.-H. KIM, J. CERN, Physics Dept. Univ. at Buffalo, SUNY, Buffalo, NY, M. CUKR, V. NOVAK, T. JUNGWIRTH, Institute of Physics, Acad. of Sciences of the Czech Republic, Prague, Czech Republic, J. SINOVÁ, Physics Dept., Texas A&M Univ., College Station, TX — We determine the complex infrared (0.1-1.2 eV) magneto-conductivity tensor of a series of Ga1−xMnx As films from the complex Faraday and Kerr angles as outlined in M.-H. Kim, et al., Phys. Rev. B 75, 214416 (2007). A systematic series of samples with varying Mn and hole concentrations is studied. The samples range from insulating to metallic. The frequency dependence of the real part of the longitudinal conductivity σxx is consistent with the values determined from transmission and reflection measurements. The complex transverse (Hall) conductivity σyz shows resonances associated with the inter-valence band transitions. As the Mn concentration decreases these transitions become broadened due to increased disorder. The temperature dependence shows non-monotonic behavior with sign changes at certain wavelengths. The data is compared with predictions from a disordered valence band model (T. Jungwirth, et al., Phys. Rev. B 76, 125206 (2007)). This work is supported by the Research Corporation Cottrell Scholar Award (Buffalo and Texas A&M), NSF-CAREER-DMR0449899 (Buffalo), an instrumentation award from the CAS, Univ. at Buffalo, ERAS-CT-2003-980409 (Prague) and NSF-CAREER-DMR-0547875 (Texas A&M).
3:42PM S33.00007 An n-type tunable two-dimensional ferromagnetic semiconductor. ANGELO BOVE, F. ALTOMARE, N. KUNDTZ, A. CHANG. Physics Department, Duke University, Durham, NC 27708. — In the past two decades ferromagnetic semiconductors have been a focus of intense study because of their potential technological application for spintronics. Particular attention has been dedicated to III-V Diluted Magnetic Semiconductors (DMS), where the ferromagnetism (FM) is hole-mediated and the Curie temperature can therefore be tuned by changing the concentration of free carriers. In these structures, the Anomalous Hall Effect (AHE) has played a key role in establishing that FM is hole-mediated. We will present data that show the first evidence of electron-mediated FM in GaMnAs. Our heterostructure has a low carrier density (\(\sim 1.1 \times 10^{12} \text{cm}^{-2}\)), a mobility of \(\sim 600 \text{cm}^2/\text{V} \cdot \text{s}\) and excellent gating capabilities. We will also present data that show the first clear bound on the AHE in an electron-mediated DMS and find it much reduced in magnitude when compared to the case of hole-mediated FM.

1Research supported in part by NSF NIRT DMR-0210519.

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3:54PM S33.00008 Electrically-induced Spin Coherence by Ultrafast Electrical Spin Injection. B. BESCHLEROß, L. SCHREIBER, J. MORITZ, C. SCHWARK, G. GUENTHERODT. Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN — Efficient electrical spin injection from a ferromagnet into a semiconductor has been demonstrated for various material systems by steady-state experiments. We introduce a novel time-resolved technique based on electrical pumping and optical probing. As a pump we apply ultrafast current pulses (\(\sim 200 \text{ps}\)) to electrically inject spin packets from an iron layer through a reverse biased Schottky barrier into a n-GaAs layer. Spin coherence in the semiconductor is probed by subsequent spin precession in a transverse magnetic field using time-resolved Faraday rotation. We observe spin precession for current pulse widths down to 200 ps. The spin polarization of the spin packets is directly measured by Faraday rotation and is found to increase linearly with the current pulse width for pulses shorter than 3 ns at small magnetic fields. This finding together with independent measurements of the samples' high frequency bandwidth indicate that even shorter than 200 ps pulses might be used for generating coherent spin currents in our devices. Work supported by BMBF, DFG and HGF.

4:06PM S33.00009 Electrical detection of spin polarized current in semiconductors using Andreev reflection. PARTHA MITRA, MENG ZHU, NITIN SAMARTH. Department of Physics, The Pennsylvania State University — Electron transport across the interface between a superconductor and a normal conductor is sensitive to the spin populations of electrons in the conduction band of the latter, leading to the phenomenon of Andreev reflection. A characteristic non-linear behavior in differential conductance is observed in superconductor/ferromagnet bilayers, with a suppression of the conductivity below the superconducting gap. This allows the carrier spin polarization in the normal conductor to be extracted. We attempt to exploit Andreev reflection for measuring hole spin diffusion lengths in p-GaAs by studying a series of hybrid heterostructures of superconducting metal (In or Nb) and a ferromagnetic semiconductor (GaMnAs), separated by p-GaAs spacer layers of different thickness. Qualitatively, our data show evidence for a finite spin polarization in the current that decreases with spacer thickness.

1Work supported by the ONR MURI program.

4:18PM S33.00010 Reconfigurable spin logic gate in Gallium Arsenide. C. AWO-AFFOUDA, O.M.J. VAN ’T ERVE, M. HOLUB, C.H. LI, A.T. HANBICKI, G. KIOSEOGLIOU, B.T. JONKER. Naval Research Laboratory, Washington, DC 20375 — Electrical injection and detection of pure spin currents has recently been shown in semiconductors. Here we concentrate on the realization of spin-based logic circuits in semiconductors. We report on the electrical injection and detection of spin polarized currents using reconfigurable magnetic contacts. Fe/GaAs Schottky contacts are used to create and analyze the spin current in a GaAs transport channel. Non-local detection techniques show that the circuit output voltage can be modulated using current carrying wires that independently switch the magnetization of the contacts. We use this effect to generate a logic function based on pure spin transport in semiconductors. The realization of this integrated spin-based structure may facilitate the development of pure spin-based logic gates.

1This work was supported by ONR and core NRL programs.

4:30PM S33.00011 Inversion of Ferromagnetic Proximity Polarization in GaAs by MgO Interlayers. Y. LI, Y. CHYE, Y.F. CHIANG, K. PI, W.H. WANG. Department of Physics and Astronomy, UC Riverside, J.M. STEPHENS, S. MACK, D.D. AVSCHALOM, Center for Spintronics and Quantum Computation, UC Santa Barbara, R.K. KAWAKAMI, Department of Physics and Astronomy, UC Riverside — Ferromagnet/semiconductor hybrid structures are building blocks for spin transport devices and spin-based logic gates for large- scale circuits. Recent experiments achieved success in making a lateral Fe/GaAs spin transport device, but anomalous bias dependence of the spin injection signal demand an understanding of the role of atomic-scale interfacial structure in determining the spin dependent reflection and transmission coefficients. In our studies, we incorporate a spin-filtering material MgO in the Fe/GaAs structure, and directly study the spin dependent reflection properties of the interface, or the ferromagnetic proximity polarization (FPP) effect, through ultrafast optical measurements. We find that the FPP in Fe/MgO/GaAs can be tuned by controlling MgO thickness, and we observe a sign change by MgO interlayers. Through study of the related nuclear spin polarization, we also observed sign change of FPP with laser intensity when MgO thickness is in the transition range of sign change. By modification of the interface, mainly changing oxygen partial pressure during MgO growth, we find that the Fe-Mg bond is a key factor in the sign change. Supported by CNID, ONR and NSF.

4:42PM S33.00012 GaMnAs-based hybrid multiferroic memory device. M. OVERBY, A. CHERNYSHOV, L.P. ROKHINSON, Department of Physics, Purdue University, West Lafayette, IN 47907, J.K. FURDYNA, X. LIU. Department of Physics, University of Notre Dame, Notre Dame, IN 46556 — In a ferromagnetic semiconductor GaMnAs grown on GaAs there are two equivalent easy axes of magnetization along the [100] and [010] crystallographic directions. These two directions can form a basis for a memory device with the binary state being encoded in the direction of the magnetization. The state can be electrostatically controlled by introducing a compressive (tensile) strain along one of the easy axes. We demonstrate a novel non-volatile hybrid multiferroic memory cell with electrostatic control of magnetization based on strain-coupled GaMnAs and a piezoelectric material. The magnetization direction is monitored via planar Hall effect, which changes sign when magnetization rotates. At zero voltage on the piezoelectric magnetization can be oriented either along [100] or [010], when voltage on piezoelectric is swept between positive and negative values magnetization forms a hysteresis loop with abrupt transitions between the two orientations.
4:54PM S33.00013 Reversal of spin polarization in Fe/GaAs (001) driven by resonant surface states: First-principles calculations, A.N. CHANTIS, Theoretical Division, Los Alamos National Laboratory, K.D. BELASHCHENKO, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, D.L. SMITH, Theoretical Division, Los Alamos National Laboratory, E.Y. TSYMBAŁ, Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, M. VAN SCHILFGAARDE, Arizona State University, R.C. ALBERS, Theoretical Division, Los Alamos National Laboratory — A minority-spin resonant state at the Fe/GaAs(001) interface is predicted to reverse the spin polarization with voltage bias of electrons transmitted across this interface. Using a Green’s function approach within the local spin density approximation we calculate spin-dependent current in a Fe/GaAs/Cu tunnel junction as a function of applied bias voltage. We find a change in sign of the spin polarization of tunneling electrons with bias voltage due to the interface minority-spin resonance. This result explains recent experimental data on spin injection in Fe/GaAs contacts [1,2] and on tunneling magnetoresistance in Fe/GaAs/Fe magnetic tunnel junctions [3].


5:06PM S33.00014 Spin-Polarized Edge-Emitting Lasers¹, M. HOLUB, A.T. HANBICKI, C.S. KIM, G. KIOSEOGLOU, O.M.J. VAN ’T ERVE, C.H. LI, I. VURGAFTMAN, J.R. MEYER, B.R. BENNETT, B.T. JONKER, Naval Research Laboratory — Semiconductor lasers driven by a spin-polarized current are expected to provide a threshold current reduction, optical polarization control, and intensity stabilization. We explore these possibilities in edge-emitting lasers where the low switching fields of in-plane magnetized Fe thin films should enable electronic modulation of the output polarization. Fe/GaAs/GaAs heterostructures are designed, grown, and fabricated into surface-emitting light-emitting diodes (LEDs) and double heterostructure lasers. The LED emission is dominated by an H-band feature at 5 K and by the bulk recombination feature at 20 K. An electron spin polarization of 24% is measured in the Faraday geometry. Oxide-stripe lasers are fabricated with and without an Fe capping layer. Lasing is observed at low temperatures with threshold current densities of ∼100 A/cm². Magnetic field-dependent studies to examine the effects of spin injection on laser performance will be discussed.

1This work is supported by ONR and core NRL programs.

5:18PM S33.00015 Spin Injection into Co₂MnAl by Optical Absorption in GaAs¹, S. ISBER, American University of Beirut, Y.J. PARK, KIST, J.S. MOODERA, MIT, D. HEIMAN, Northeastern University — Ferromagnet-semiconductor heterostructure devices have been made with half-metallic ferromagnets, which have larger spin polarizations than transition metal based ferromagnets. Spin-polarized electrons generated in the semiconductor by circularly polarized light are injected across a Schottky barrier into the ferromagnet and detected as photocurrent. In this technique, the optically pumped semiconductor is the source of spin polarized electrons, and the ferromagnet is the detector of spin polarized electrons. The heterostructures consist of MBE-grown Co₂MnAl Heusler ferromagnets which are lattice matched to n⁺GaAs, forming a Schottky barrier. A magnetic field is applied parallel to the light and perpendicular to the ferromagnetic layer, allowing the magnetization to be switched from parallel to antiparallel to the light direction, thus switching the direction of the detected spin polarization. Spin-dependent photocurrent was measured as a function of applied voltage bias across the Schottky barrier. The injection of spin-polarized electrons was determined after subtracting the magnetic circular dichroism (MCD) effect.

1Research supported by the NSF Grant DMR-0305360. We thank the Arab Fund for Economic and Social Development for supporting S.I.

Wednesday, March 12, 2008 2:30PM - 5:30PM – Session S35 FIAP: Focus Session: Nanotechnology I Morial Convention Center 227

2:30PM S35.00001 Deep UV Pattern Definition in PMMA, BRIAN BURKE, TIMOTHY HERLIHY, ANDREW SPIKAS, KEITH WILLIAMS, University of Virginia — We have patterned polymethyl methacrylate (PMMA) resist by exposing it with the fifth harmonic (213 nm) of an Nd:YAG source through metallized apertures in contact with the resist. Interface patterns with both near- and far-field origins were observed. In order to test the contrast and uniformity of exposure, we deposited germanium onto developed areas to form arrays with feature sizes of approximately 200 nm. We present a straightforward model for interference effects generated in our process, and discuss opportunities for direct-write lithography through single apertures.

2:42PM S35.00002 Low Temperature Growth of ZnO Nanorods by Chemical Bath Method, MATT BAUMER, PARAMESWAR HARI, DARYL SPENCER, University of Tulsa — ZnO nanorods grown by chemical bath deposition (CBD) methods are of great interest in photonic and electronic device applications because they offer low cost, low temperature techniques compared to conventional vapor deposition and sputtering methods. Our past studies of ZnO nanorods were grown by CBD on indium tin oxide (ITO) coated glass substrates employed heating of an equimolar solution of Zinc (II) nitrate and hexamethylenetetramine solution at 95 C. Morphology of ZnO nanorods exhibited both open and closed hexagonal shape under various deposition conditions at or above 95 C. Currently we are studying the effect substrates on the morphology of the nanorods grown by chemical bath technique. We are using glass coated with tin oxide, aluminum, as well as solid molybdenum as substrates. We will use scanning electron microscopy and atomic force microscopy to map the changes in morphology of nanorods grown on various substrates. We will present quantitative data on changes in cluster size and shape of nanorods as the growth substrate is varied.

2:54PM S35.00003 Nano-assembly and Controlled Release Kinetics of Nanoelements from Nanoporous Templates, E. GULTEPE, D. NAGESHA, J. MCNULTY, S. SRIDHAR, eMRI, Dept. of Physics and Nanomedicine Consortium, Northeastern University — Nanotemplates and nanoparticle成長 potential for use in the area of nanomanufacturing and biomedical applications. We are using highly ordered nanoporous alumina as a template for drug delivery and to assemble nanoelements such as latex beads and single wall carbon nanotubes (SWNT) by the means of electrophoresis and/or dielectrophoresis. The results of 100% assembly of latex beads and controlled elution of drugs from nanoporous templates will be discussed. Vertically assembled SWNT and I-V characteristic as 3D interconnects, will also be presented. We have developed a variety of platforms incorporating superparamagnetic iron oxide nanoparticles for targeted delivery, magnetic hyperthermia and as a contrast agent for magnetic resonance imaging. The results of cell studies on these platforms will be discussed.

1This work was supported by the National Science Foundation (NSF) IGERT Nanomedicine Science and Technology (NSF-0504331) and NSF Nanoscale Science and Engineering Centers Program (NSF-0425826).
on the nanowire mat about showed reversible response to CO exposure. The sensor is a two-terminal design, where the terminals consist of two 25 \( \mu \)m of ZnO nanostructures. Here, we report the electrical properties of a gas sensor constructed from mats of ZnO nanowires grown on sapphire substrate that were produced by a conventional mechanical test. The presence of the nanowires is directly related to the one-dimensional meniscus configuration with a small viscosity at high temperatures and to the wide supercooled liquid region of the metallic glass. The electron microscopic observations demonstrate the diameters, the lengths, and the dimorphs in structural states, and the energy dispersive X-ray reveals the chemical components. In addition, we found that round ridges are constructed from nanotubes. The finding of amorphous nanostructures provides not only fundamental understanding of fracture processes but also give a new insight into nano-science and engineering.

ZHANG, California State University, Fresno, CHRIS BERVEN, University of Idaho — In the past decade, significant advances have been made in the synthesis of ZnO nanostuctures. Here, we report the electrical properties of a gas sensor constructed from mats of ZnO nanowires grown on sapphire substrate that were produced by a conventional mechanical test. The presence of the nanowires is directly related to the one-dimensional meniscus configuration with a small viscosity at high temperatures and to the wide supercooled liquid region of the metallic glass. The electron microscopic observations demonstrate the diameters, the lengths, and the dimorphs in structural states, and the energy dispersive X-ray reveals the chemical components. In addition, we found that round ridges are constructed from nanotubes. The finding of amorphous nanostructures provides not only fundamental understanding of fracture processes but also give a new insight into nano-science and engineering.

The dynamics of the deposition of nanotubes under different CMOS compatible manufacturing conditions was modeled using 2D and 3D finite element analysis. Bell Laboratories — The accurate positioning of an individual vertically aligned carbon nanotube (CNT) is a challenge for nanofabrication. We have successfully deposited individual CNT’s into sub-100nm diameter SiN windows on metal interconnects using electrophoresis in conjunction with the nanoscopic lens effect. The dynamics of the deposition of nanotubes under different CMOS compatible manufacturing conditions was modeled using 2D and 3D finite element analysis. Surface charge accumulation and saturation is the key determinant of the strength of the nanoscopic lens. The modeling predicts that there is an easily obtainable range of conditions where only one nanotube will be deposited in round windows using current generation lithography. Deposition in a slotted window geometry yields a limited number of nanotubes that have an average spacing which is a function of the geometry of the slot and randomly approaching nanotubes. Early integration of vertical carbon based logic with CMOS is feasible.

3:06PM S35.00004 Ionic PN and PNP junctions – Diodes and Transistors, ERIC KALMAN, UC Irvine, IVAN VLASTIOUK, PAVEL APEL, ZUZANNA SIWY — There are well-known devices for controlling the transport of electrons, but very few control ions in a solution. We have prepared ionic diodes and transistors that function in a similar manner to their semiconductor analogues. Ionic PN junctions were created by surface patterning single conical nanopores in polymer films, so that the pore walls are split into two sections: one with positive charge, and the other with negative. These diodes can achieve rectification degrees of several hundreds. Ionic PNP junctions were created by surface patterning single double-conical nanopores in polymer films with tip diameters between 2 and 6 nm, so that the pore walls are split into three sections: the two areas near the large pore openings which are positively charged, while the center of the pore, near the pore tip, is negatively charged. This device works in a similar fashion to a semiconducting BJT transistor, and we show that we can control the electric potential chemically in a manner sufficient to gate the ion current through the device.

3:18PM S35.00005 Metallic glass nanowire, KOJI NAKAYAMA, Tohoku University, YOSHIHIKO YOKOYAMA, GUOQIANG XIE, QINGSHENG ZHANG, MINGWEI CHEN, TOSHIO SAKURAI, AKIHISA INOUE — Metallic glass nanowires were spontaneously created on the fracture surfaces that were produced by a conventional mechanical test. The presence of the nanowires is directly related to the one-dimensional meniscus configuration with a small viscosity at high temperatures and to the wide supercooled liquid region of the metallic glass. The electron microscopic observations demonstrate the diameters, the lengths, and the dimorphs in structural states, and the energy dispersive X-ray reveals the chemical components. In addition, we found that round ridges are constructed from nanotubes. The finding of amorphous nanostructures provides not only fundamental understanding of fracture processes but also give a new insight into nano-science and engineering.

3:30PM S35.00006 CO Gas Sensing with ZnO Nanowire Mat, SIRISHA CHAVA, University of Idaho, DAQING ZHANG, California State University, Fresno, CHRIS BERVEN, University of Idaho — In the past decade, significant advances have been made in the synthesis of ZnO nanostructures. Here, we report the electrical properties of a gas sensor constructed from mats of ZnO nanowires grown on sapphire substrate that were produced by a conventional mechanical test. The presence of the nanowires is directly related to the one-dimensional meniscus configuration with a small viscosity at high temperatures and to the wide supercooled liquid region of the metallic glass. The electron microscopic observations demonstrate the diameters, the lengths, and the dimorphs in structural states, and the energy dispersive X-ray reveals the chemical components. In addition, we found that round ridges are constructed from nanotubes. The finding of amorphous nanostructures provides not only fundamental understanding of fracture processes but also give a new insight into nano-science and engineering.

3:42PM S35.00007 Mechanical Properties of Nanometric Wire of Water, MANHEE LEE, BAEKMAN SUNG, WONHO JHE, Department of Physics and Astronomy, Seoul National University, Seoul 151-742, Korea, CNL TEAM — Water has been one of the perfect newtonian viscosious liquids, which are exactly described by navier-stokes equations. Recently, it, however, was found that the effective shear viscosity of water confined between mica crystals at 10nm thickness is very different from the one of 3-dimensional bulk water. While some researchers have measured very high viscoelasticity of the confined liquid, the other researchers reported the fluidic nature of water confined between mica surfaces at <3.5 nm interfacial separation (bulk-like water-viscosity). These conflicting results concerning the mechanical properties of nanometric water have been continually reported for the past several years. None of them clearly clarified the mechanical properties of nanometric water, and the detailed behavior of the viscoelasticity within a tip-sample separation less than 1 nm has not been measured. We present the mechanical properties of nanometric water with a spatial resolution less than 0.1nm such as viscoelasticity, dissipation energy, and phase transitions.

3:54PM S35.00008 Growth of Vertically Aligned Carbon Nanotube on Glass, TRILOCHAN PAUDEL, JAKUB RYBCZYNSKI, ZHIFENG REN, BOSTON COLLEGE TEAM — Periodic arrays of vertically aligned carbon nanotubes on glass have been grown by dc plasma enhanced chemical vapor deposition on patterned Nickel dots prepared by polystyrene nanosphere lithography. A thin buffer layer of Titanium was first coated on cleaned high temperature C1737 Aluminosilicate glass substrates and then a monolayer of self-assembled polystyrene buffer layer of Titanium was first coated on cleaned high temperature C1737 Aluminosilicate glass substrates and then a monolayer of self-assembled polystyrene spheres was deposited on the glass. Through the polystyrene spheres, a hexagonal pattern of triangular Nickel dots was obtained after removing the spheres. The sphere size and Nickel thicknesses consequently determine the diameter and the site density of carbon nanotubes. The successful growth of carbon nanotubes on glass substrates with good periodicity and alignment are crucial to bio-sensor and solar cell applications.

4:06PM S35.00009 Feedback Cooling of a Massive Resonator, Quartz Tuning-fork, in Air, BAEKMAN SUNG, MANHEE LEE, WONHO JHE, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, CNL TEAM — Recently, the cooling of a mechanical resonator through active feedback control has been interested for many researchers and the experiment for a cantilever cooling by using a resonator in an air control [1]. While the recent cooling experiments have been done by tiny cantilever in vacuum, we performed the feedback cooling experiment in air by using a very massive harmonic oscillator, a tuning fork, which has been used as an useful force sensor due to its high stiffness and dynamic oscillation property in scanning probe microscopy (SPM) such as near field scanning optical microscopy, atomic force microscopy (AFM) [2]. This technique is expected to study the low temperature micro scale effect of macroscopic object in air. // [1] M.Poggio, C.L.Degen, H.J.Mamim, and D.Rugar, PRL 99,017201 (2007). [2] F. J. Giessibl, S. Hembacher, M. Herz, Ch. Schiller, and J. Mannhart, Nanotechnology 15, S79 (2004).

4:18PM S35.00010 Molecular quantum-dot cellular automata–from molecular structure to circuit dynamics, YUHUI LUI, CRAIG LENT, Unv. of Notre Dame — Quantum-dot cellular automata (QCA) [1] provides a transistor-less paradigm for molecular electronics. In the QCA approach, binary information is stored in the charge configuration of single cells, and transferred via Coulomb coupling between neighboring cells. Single-molecule QCA cells can be realized by using as quantum dots the localized states of mixed-valence complexes. Several candidate QCA molecules have been synthesized and shown to have the required field-induced switching properties [2]. We report progress towards a hierarchic dynamic theory of QCA circuits. We use ab initio techniques to calculate the relevant molecular electronic structure, and extract parameters for a simpler Hamiltonian to describe switching behavior. We then apply a coherence formalism to model interaction with the thermal environment and generate a circuit-dynamic description. [1] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, Nanotechnology, vol. 4, pp. 49, 1993. [2] H. Qi, S. Sharma, Z. Li, G. L. Snider, A. O. Orlov, C. S. Lent, and T. P. Fehlner, J.Am.Chem.Soc., vol. 125, pp. 15250, 2003.

4:30PM S35.00011 Theory of Individual Carbon Nanotube Deposition by Nanoscopic Lenses, SHENG LIU, AMIT GOYAL, ZAFAR IQBAL, GORDON A. THOMAS, REGINALD C. FARROW, New Jersey Institute of Technology, LINUS A. FETTER, Bell Laboratories — The accurate positioning of an individual vertically aligned carbon nanotube (CNT) is a challenge for nanofabrication. We have successfully deposited individual CNT’s into sub-100nm diameter SiN windows on metal interconnects using electrophoresis in conjunction with the nanoscopic lens effect. The dynamics of the deposition of nanotubes under different CMOS compatible manufacturing conditions was modeled using 2D and 3D finite element analysis. Surface charge accumulation and saturation is the key determinant of the strength of the nanoscopic lens. The modeling predicts that there is an easily obtainable range of conditions where only one nanotube will be deposited in round windows using current generation lithography. Deposition in a slotted window geometry yields a limited number of nanotubes that has an average spacing which is a function of the geometry of the slot and randomly approaching nanotubes. Early integration of vertical carbon based logic with CMOS is feasible.

1Work supported by DARPA and AFOSR.
2Corresponding author.
include the generally low H \(_2\) adsorption uptake. To improve the H \(_2\) adsorption affinity in MOFs, our previous work has shown that the coordinatively unsaturated adsorption sites in a Cl-MOF as an example, here we show that the H\(_2\) binding with the exposed TM site is not of the expected Kubas type, in strong contrast to "similar" ion−metal interactions. We also study the H\(_2\) binding with Mn-\(d\) orbitals and find no evidence of any H\(_2\)-\(σ^*\)-Mn orbital hybridization. We also study the H\(_2\) binding as a function of Mn-\(σ\) magnetic spin configurations, and find no significant effect of the magnetic state on the binding energy. We further reveal that the major contribution to the overall binding is classical Coulomb interaction arising from the small charge overlap of H\(_2\)-\(σ\) and Mn-\(d\) orbitals. This coulomb interaction is very anisotropic, and when the quantum nature of H\(_2\)-orientation is taken into account, the actual binding energy is significantly reduced from the calculated classical binding energy. [1] J. Am. Chem. Soc. 128, 16876 (2006).

4:42PM S35.00012 CMOS based fabrication of single electron devices on a large scale. VISHVA RAY, RAMKUMAR SUBRAMANIAN, PRADEEPI BHADRACHALAM, SEONG JIN KOH, The University of Texas at Arlington — Fabrication of single electron devices requires device components (a Coulomb island, source and drain electrodes) to be arranged with nanoscale precision. This has been so far carried out utilizing techniques such as e-beam lithography, shadow evaporation, electromigration, and scanning probe microscopy, which are not suitable for large-scale fabrication for practical use. Here we present new single electron device architecture and its large-scale fabrication within the framework of CMOS fabrication technology. This has been done by employing vertical electrode configuration where the source and drain electrode separation is controlled with nanoscale precision over an entire wafer. Colloidal Au nanoparticles of 10-20 nm diameter were used as Coulomb islands positioned between the source and drain electrodes. We observed clear Coulomb blockade and Coulomb staircase at room temperature for 10 nm Au nanoparticles with charging energies of ~50 meV, in good agreement with self-capacitance values of 10 nm Au particle. The experimental I-V characteristics also agree well with simulated I-Vs carried out using the orthodox theory.

4:54PM S35.00013 A QCM study of the dynamics and frictional properties of physisorbed polysytrene microspheres on a Au(111) Surface\(^1\), IYAM LYNCH, JACQUELINE KRIM, North Carolina State University, JESSICA MCNUTT, University North Carolina Asheville — The notion of transporting micro/nano objects has been of interest to the scientific community since the early days of nanotechnology. Progress in this area requires an understanding of the frictional behavior of these objects when they are in motion. In this study we have analyzed the behavior of 5μm diameter polysyrene spheres physisorbed on the electrode of a quartz crystal microbalance (QCM) in orientations normal and parallel to gravity. By varying the driving voltage of the QCM, the samples exhibit a frequency response with respect to the crystal amplitude ("decoupling curve"). This decoupling curve gives information about the motion of the spheres on the surface and leads to the calculation of the particles sliptime which gives rise to the frictional forces between the particles and surface. Optical observations show that the particle motion is dependent on the oscillation direction of the QCM and gravity to a lesser extent. Quantitative comparisons of the friction force and the optically observed sliding motion have been performed and will be reported on.

\(^1\) NSF and NTC are thanked for their support.

5:06PM S35.00014 Dynamic behavior of inter-pulse timing intervals of neuron-like pulses in a GaAs/InGaAs multi-quantum well structure.\(^2\), ARUNA WEERASEKARA, STEVEN MATSUK, GENNADY CYMBALYUK, A. G. UNIL PERERA, Georgia State University — Neuron-like triggered pulses in a GaAs/InGaAs multi-quantum well (MQW) structure, which shows an s-type negative differential resistance (SNDR), was investigated. Dynamic behavior of inter-pulse timing intervals (IPTIs) was studied by analyzing first return maps, power spectra, and correlation dimensions. First return maps of the IPTIs show an interesting grouping pattern at slower pulse rates. The grouping behavior can be empirically modeled using oscillatory behavior of the pulsing threshold level of the MQW structure. This pattern of IPTIs is similar to that of thermoreceptors in fish and mammals. Under different operational conditions, correlation dimension of 8.0, 8.5, and 10.0 were obtained by calculating the correlation integrals. The obtained correlation dimensions suggest that this system possesses a higher dimensional behavior.

\(^2\) This work is partially supported by GSU Brain and Behavior Program

5:18PM S35.00015 Using a quantum point contact as a sensitive detector of cantilever motion. M. POGGIO, M.P. JURA, C.L. DEGEN, M.A. TOPINKA, H.J. MAMIN, D. GOLDBERG-GORDON, D. RUGAR, IBM RESEARCH DIVISION, ALMADEN RESEARCH CENTER, 650 HARRY RD., SAN JOSE, CA COLLABORATION, CENTER FOR PROBING THE NANOSCALE, STANFORD UNIVERSITY, 476 LOMITA HALL, STANFORD, CA COLLABORATION — We demonstrate the use of a GaAs quantum point contact (QPC) as a sensitive displacement detector with the ability to resolve the thermal motion of an ultrasoft micromechanical oscillator. The displacement measurement is made by positioning the tip of a metal-coated Si cantilever ~100 nm above a QPC. The application of a small voltage to the lever causes it to gate the conductance through the QPC. As a result, motion of the cantilever’s tip modulates the conductance. By measuring this modulation, we achieve a displacement resolution better than 10-12 m/Hz\(^{1/2}\), which is comparable to the resolution achieved by low power optical interferometry. The flexibility of an on-chip QPC as a sensor of cantilever displacement has a number of potential applications including magnetic resonance force microscopy, the detection of displacement for cantilevers with dimensions smaller than the optical diffraction limit, and the cooling of mechanical resonators through feedback.

Wednesday, March 12, 2008 2:30PM - 5:30PM –
Session S36 DMP FIAP: Focus Session: Hydrogen Storage III: Novel Porous and Sorbent Materials Morial Convention Center 228

2:30PM S36.00001 Enhancing the interaction strength and capacities of hydrogen storage via surface adsorption. CRAIG BROWN, NIST Center for Neutron Research — Storing Hydrogen molecules in porous media based on a physisorption mechanism is one possible approach to reach the US Department of Energy targets for on-board hydrogen storage. Although the storage capacities of metal centers (CUMCs) can greatly enhance the H\(_2\) storage capacity, this has been done by employing vertical electrode configuration where the source and drain electrode separation is controlled with nanoscale precision over an entire wafer. Colloidal Au nanoparticles of 10-20 nm diameter were used as Coulomb islands positioned between the source and drain electrodes. We observed clear Coulomb blockade and Coulomb staircase at room temperature for 10 nm Au nanoparticles with charging energies of ~50 meV, in good agreement with self-capacitance values of 10 nm Au particle. The experimental I-V characteristics also agree well with simulated I-Vs carried out using the orthodox theory.

3:06PM S36.00002 Nature of the Hydrogen Binding in Metal Organic Frameworks with Exposed Transition Metal Sites. WEI ZHOU, NIST and UMD, TANER YILDIRIM, NIST and UPENN — MOFs with exposed transition metal (TM) sites were recently found to exhibit significantly larger experimental heat of H\(_2\) adsorption than classical MOFs, thus attracted great attention. [1, 2] Understanding the nature of the H\(_2\) interaction with the exposed metal sites is of critical importance for the further development of these materials. Using Mn-Cl-MOF as an example, here we show that the H\(_2\) binding with the exposed TM site is not of the expected Kubas type, in strong contrast to "similar" systems investigated previously (e.g., ref. [3] and [4]). In Mn-Cl-MOF, there are a) no charge transfer from TM to H\(_2\), b) no significant H-H bond elongation, and c) no evidence of any H\(_2\)-\(σ^*\)-Mn orbital hybridization. We also study the H\(_2\) binding as a function of Mn-\(σ\) magnetic spin configurations, and find no significant effect of the magnetic state on the binding energy. We further reveal that the major contribution to the overall binding is classical Coulomb interaction arising from the small charge overlap of H\(_2\)-\(σ\) and Mn-\(d\) orbitals. This coulomb interaction is very anisotropic, and when the quantum nature of H\(_2\)-orientation is taken into account, the actual binding energy is significantly reduced from the calculated classical binding energy. [1] J. Am. Chem. Soc. 128, 16876 (2006).
3:18PM S36.00003 Kinetic and steric differences in adsorption in two porous metal-organic frameworks. KATHLEEN LASK, VAIVA KRUNGLEVICTE, MURAT BULUT, ALDO MIGONE, Southern Illinois University, J.-Y. LEE, JING LI, Rutgers University — Kinetic and steric differences are two of the three fundamental mechanisms underlying the use of adsorption in applications to gas mixture separations. We present experimental results on kinetics and equilibrium adsorption measurements of tetrafluoromethane and argon on two metal-organic framework (MOF) materials: RPM1-Co or [Co3(bpdc)3(bpy)]·4DMF·H2O (bpdc = biphenyldicarboxylate, bpy = 4,4′-bipyridine, DMF = N,N′-dimethylformamide) and Cu-BTC or Cu2[BTC]2·(H2O)3 (BTC = benzene-1,3,5-tricarboxylate). The adsorbates display significant differences in their kinetics on RPM1-Co (i.e., there are sizable differences in the time required for each gas to reach equilibrium after it is allowed access to the substrate). Our equilibrium measurements show that CF4 is sterically precluded from adsorbing in the small tetrahedral-shaped side pockets present in Cu-BTC. We will compare our experimental results with predictions for how adsorption kinetics depends on the size of the adsorbate and on those of the pores present in the substrate.

3:30PM S36.00004 A theoretical and experimental study of hydrogen storage in metal organic framework materials. VALENTINO R. COOPER, JEONG YONG LEE, JING LI, YVES CHABAL, DAVID C. LANGRETH, Rutgers University — Metal-organic framework (MOF) materials, assembled by linking metal ions or clusters through molecular bridges, have been shown to be good candidates for H2 storage. We have been successful in fabricating and characterizing MOFs with increased H2 uptake though still too low for commercial applications. Here we present a coordinated theoretical-experimental effort to understand the mechanism of H2 adsorption in true MOF materials. Using the completely ab initio van der Waals density functional (vdW-DF), we simulate the interactions of H2 within Zn2(bdc)$_2$(tead). We demonstrate that modeling the entire MOF structure can result in different H2 adsorption geometries, binding energies and vibrational frequencies than observed in calculations on fragments of the MOF. Combining these results with experimental IR vibrational frequency studies may provide insights into modifying MOF structure and composition for enhanced H2 uptake. 

3:42PM S36.00005 The flexibility of zeolites for Hydrogen storage. ASEL SARTBAEVA, Oxford University, STEPHEN ANTHONY WELLS, Warwick University, PETER P. EDWARDS, Oxford University — The flexibility window is a newly discovered theoretical measure which can provide a valuable selection criterion when evaluating hypothetical zeolite framework structures as potential synthetic targets. Today synthetic zeolites are the most important catalysts in petrochemical refineries. There have been considerable efforts to synthesize new zeolites with specific pore geometries, to add to the 167 available at present. Millions of hypothetical structures have been generated on the basis of energy minimization, and there is an ongoing search for criteria capable of predicting new zeolite structures. The flexibility window appears to be a property of existing zeolite frameworks not shared by many hypothetical structures. It provides a valuable selection criterion when evaluating hypothetical zeolite framework structures as potential synthetic targets. We are investigating the use of zeolites as hydrogen storage materials, as small molecules such as molecular hydrogen and ammonia can be easily absorbed into a flexible framework of zeolites. An exiting possibility is the use of framework flexibility to control hydrogen uptake, storage and release. This would allow a safe use of hydrogen for fuel cells.

3:54PM S36.00006 Inelastic Incoherent Neutron Scattering Studies of the Ti-doped hydrogen-adsorbed SBA-15. ALICE I. ACATRINEI, LUKE L. DAEMEN, MONIKA A. HARTL, Los Alamos National Laboratory, LANSCE-LC — The discovery in 1998 of the hydrothermally stable SBA-15 by Zhao et al. [1] represents a great advance in the synthesis of ordered mesoporous materials. The high porosity, good thermal stability, and low specific weight of these materials makes them good candidates for hydrogen storage research, and metal doping shows an enhancement of their properties and gas storage capabilities. We used inelastic incoherent neutron scattering to look at both Ti-doped and undoped hydrogen adsorbed SBA-15. Powder XRD measurements confirmed the mesoporosity of the material. Adsorption isotherm showed that a significant amount of hydrogen was adsorbed in the compound. Our results indicate that hydrogen binds to the Ti centers in the material. [1]. D. Zhao, J. Feng, Q. Huo, N. Melosh, G.H. Fredrickson, B.F. Chmelka, G.D. Stucky, Science 279 (1998) 548.

4:06PM S36.00007 Hydrogen Storage in Mesoporous Materials under High Pressure. MICHELLE WEINBERGER, MADDURY SOMAYAZULU, RUSSELL HEMLEY, Geophysical Lab, Carnegie Institution of Washington — To date, the materials considered best candidates for hydrogen storage fuel cells include activated carbon and metal organic frameworks. Both very high surface area activated carbon and MOF-S have been shown to adsorb around 4.5 wt % of hydrogen gas at 78 K. We have investigated the fundamental structural response of these materials to high pressure, as well as their behavior at high pressure when packed with dense hydrogen. Further investigation of these materials at low temperatures while still at elevated pressures may in fact provide a route for recovery of these hydrogen-packed materials to near ambient conditions. Covalent organic frameworks offer the potential for even better hydrogen storage capacity. These materials have significantly lower densities than the MOF materials and offer a significantly larger number of adsorption sites. Diamond anvil cells are uniquely suited for the study of these materials, allowing in situ measurements at high pressure as well as at low temperatures. Using X-ray diffraction and Raman spectroscopy and Infrared Spectroscopy we probe the behavior of the hydrogen confined in these porous materials at high pressure by tracking changes in the in situ high pressure x-ray diffraction patterns and shifts in the hydrogen vibrion peaks.

4:18PM S36.00008 A combined pressure-temperature synthesis approach towards novel hydrogen storage materials1. RAJA CHELLAPPA, MADDURY SOMAYAZULU, VIKTOR STRUZHKIN, RUSSELL HEMLEY, Carnegie Institution of Washington — There is a growing need to explore synthesis of novel hydrogen storage materials with very high hydrogen content (> 30 wt.%) as well as tuning materials in order to facilitate reversible hydrogen desorption and absorption. A combined pressure-temperature (P − T) approach holds considerable promise towards achieving these objectives. In this talk, we will present results from our on-going efforts to synthesize hydrogen clathrates with very high hydrogen content that can be recovered at moderate P − T conditions based on simple molecular systems including clathrates and van der Waals compounds, specifically H2O, CH4, NH3, and boron containing systems. The use of suitable additives to enhance stability will also be explored. Results will also be presented from the direct P − T synthesis of metastable light metal (Li, Mg, B-based) complex hydrides.

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1 We thank the financial support of US Department of Energy (USDOE) grants DE-FG-02-06ER46280.
4:30PM S36.00009 Structure of Nanoporous Biocarbon for Hydrogen Storage as Determined by Small Angle X-Ray Scattering. MIKAEL WOOD, J. BURRESS, J. POBST, S. CARTER, P. PFEIFER, C. WEXLER, University of Missouri-Columbia, Department of Physics, P. SHAH, G. SUPPES, University of Missouri-Columbia, Department of Chemical Engineering — As a member of the Alliance for Collaborative Research in Alternative Fuel Technology (ALL-CRAFT) our research group studies the properties of nanoporous biocarbon, produced from waste corn cob, with the goal of achieving the Department of Energy’s gravimetric and volumetric standards for both hydrogen and methane gas storage. Small Angle X-Ray Scattering (SAXS) is a valuable tool in our investigation of the geometry of the pore space in our carbon samples. In this talk, we will compare the experimental SAXS data with theoretical results for various pore geometries to determine which pore models are consistent with experiment. Using data from nitrogen adsorption isotherms, along with SAXS, yields significant structural information about the pore space. This analysis allows us to fully optimize our production process and to achieve the DOE’s target storage capacities. This work supported by: 1. National Science Foundation (PFI-0438469) 2. U.S. Department of Education (P200A040038) 3. U.S. Department of Energy (DE-AC02-06CH11357) 4. University of Missouri (RB-06-040) 5. U.S. Department of Defense (N00164-07-P-1306) 6. U.S. Department of Energy (DE-FG02-07ER46411)

4:42PM S36.00010 High Capacity Hydrogen Storage on Nanoporous Biocarbon1. JACOB BURRESS, MIKAEL WOOD, MICHAEL GORDON, University of Missouri-Columbia, PHILLIP PARILLA, NREL, MICHAEL BENHAM, Hiden Isochema, CARLOS WEXLER, FRED HAWTHORNE, PETER PFEIFER, Univ. of Missouri-Columbia — The Alliance for Collaborative Research in Alternative Fuel Technology (http://all-craft.missouri.edu) has been optimizing nanoporous biocarbon for high capacity hydrogen storage. The hydrogen storage was measured gravimetrically and volumetrically (Sievert’s apparatus). These measurements have been validated by NREL and Hiden Isochema. Sample S-33/k, our current best performer, stores 73.91 g H2/kg carbon at 77 K and 47 bar, and 1.0-1.6 g H2/kg carbon at 293 K and 47 bar. Hydrogen isotherms run by Hiden Isochema have given experimental binding energies of 8.8 kJ/mol compared to the binding energy of graphite of 5 kJ/mol. Results from a novel boron doping technique will also be presented. The benefits and validity of using boron-doping on carbon will also be discussed.

1Optimal pore sizes and volumes will be presented for hydrogen storage nanoporous carbon.

4:54PM S36.00011 Preparation and Cryogenic Hydrogen Storage Capacity of Nanoporous Carbon Materials Synthesized using an Aerosol-Assisted Approach. QINGYUAN HU1, Purdue University, YUNFENG LU, Univ. Cal. Los Angeles, GREGORY P. MEISNER, GM Research and Development Center — Spherical nanoporous carbon particles were synthesized from carbon precursor solutions of sucrose with either silica sols, colloidal silica particles, or both, in a direct one-step aerosol-assisted process, followed by carbonization and then removal of the silica template. The resulting particles show very high porosity with narrow pore size distributions, surface areas up to 2000 m2/g, and pore volumes up to 4.0 cm3/g. The porosity and pore sizes depend on the type and amount of silica template precursor added to the sucrose precursor solutions. The carbon particles were characterized by transmission electron microscopy, field emission scanning electron microscopy, and nitrogen sorption surface area measurements. Hydrogen adsorption was measured at various temperatures between 77 K and room temperature and at pressures up to 50 bars. The maximum hydrogen uptake of up to 4.0 wt% at 77 K and >20 bar was found for nanoporous carbon particles made using the silica sol template.

5:06PM S36.00012 NMR Characterization of Hydrogen Adsorption and Pore Structures of Carbon-Based Materials1. B.J. ANDERSON, ALFRED KLEINHAMMES, YUE WU1, Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC 27599-3255, UNIVERSITY OF PENNSYLVANIA DEPARTMENT OF CHEMISTRY COLLABORATION, LAWRENCE LIVERMORE NATIONAL LABORATORY COLLABORATION — Hydrogen adsorption in carbon-based materials such as boron-doped graphite and carbon aerogels was investigated by nuclear magnetic resonance (NMR). 1H NMR is shown to be a sensitive and quantitative probe for detecting adsorbed gas molecules such as H2, methan, and ethane. NMR measurements were carried out in-situ under given H2 pressure up to a pressure of over 100 atm, at room temperature and 100 K. From such 1H NMR measurement, the amount of adsorbed H2 molecules was determined versus pressure. In addition to measuring adsorption binding energies via isotherms, the structure and distribution of the nanopores within the material were characterized in order to relate the size of the pores to the rate of diffusion of the H2 to the adsorption sites.

1Funded by the DOE Carbon-based Hydrogen Sorption Center of Excellence, the UNC Institute for the Environment and the UNC Institute for Advanced Materials, Nanoscience and Technology

Principle Investigator

5:18PM S36.00013 Fabrication Procedures and Material Properties of Activated Carbon for Hydrogen and Methane Storage1. JEFFREY POBST, JACOB BURRESS, MIKAEL WOOD, MATTHEW BECKNER, PARAG SHAH, MICHAEL GORDON, Univ. of Missouri-Columbia, PHILLIP PARILLA, NREL, SARAH BARKER, SARA CARTER, LAUREN ASTON, GALEN SUPPES, PETER PFEIFER, Univ. of Missouri-Columbia — The Alliance for Collaborative Research in Alternative Fuel Technology (http://all-craft.missouri.edu) has developed nanoporous biocarbons with interesting pore characteristics. These carbons are being optimized for hydrogen and methane vehicular storage. Our current best performer stores 73-91 g H2/kg carbon at 77 K and 47 bar, and 1.0-1.6 g H2/kg carbon at 293 K and 47 bar. The validity of using methane storage as a predictor for hydrogen storage will be presented. Recent carbons have achieved porosities as high as of 0.8 and BET surface areas of 3,500 m2/g. Optimal pore sizes and volumes will be presented for hydrogen storage nanoporous carbon.

1NSF-PFI (PFI-0438469); GAANN U.S. Dept. of Ed. (P200A040038); D.O.E. (DE-AC02-06CH11357); MU Research Board: Univ. of Missouri (RB-06-040); D.O.D. (N00164-07-P-1306); D.O.E. (DE-FG02-07ER46411)

Wednesday, March 12, 2008 2:30PM - 5:30PM
Session S37 DCMP: Effect of Strain on Ferroelectrics Morial Convention Center 229

2:30PM S37.00001 First-principles study of novel routes to ferroelectricity using strain. ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — We use first-principles density functional theory (DFT) to explore the use of strain to induce ferroelectricity in otherwise non-polar materials. First, we investigate the polarization induced in LaAlO3 by changing in-plane bondlengths while constraining the unit cell to tetragonal symmetry. We then relax the symmetry constraint to examine the effect of oxygen octahedra rotations on the polarization. Next we explore whether epitaxial strain in the pseudocubic [100] direction can lift the inversion center in otherwise centrosymmetric BiMnO3 and induce the small polarization reported in thin films. By studying these systems with DFT calculations, we have the ability to finely vary the system constraints, predicting new functional materials and providing insight into the underlying physics.
quasirandom structures. In agreement with the literature, 
(PZT) depend upon epitaxial strains ranging from epitaxial strain, which is controlled by substrate selection. Here, using ab initio interest in ferroelectric perovskite thin films, alloys, and superlattices. Engineering of FeRAMs requires the control of both the spontaneous polarization and dielectric constant on strain will be discussed in terms of a theoretical model of the phenomenological thermodynamics of the film strain effect.

BILT, Rutgers University — The potential for creating ferroelectric-based devices such as ferroelectric random-access memories (FeRAMs) has led to an intense engineering oxide films. Work supported by the U. S. Department of Energy under Contract No. DE-AC02-06CH11357.

3:06PM S37.00004 In situ LEED-IV characterization of polar distorted ultra-thin BaTiO3 films VON BRAUN NASCIMENTO, E. WARD PLUMMER, University of Tennessee, JUN-SOO SHIN, A.Y. BORISEVICH, ARTHUR P. BADDORF, SERGEI V. KALININ, Oak Ridge National Laboratory — Ferroelectric phase stability in nanoscale ferroelectrics is governed by the interplay of electrostatic depolarization energy, domain formation, adsorption, and surface band bending. Predictions for the minimum critical film thickness for ferroelectricity in BaTiO3 have continuously decreased with more complex models to a current value of 6 layers. The thinnest experimental value is 12 layers. Using in situ low energy electron diffraction (LEED) - IV, we have characterized the structure of 4 and 10 ML BaTiO3 films, grown using molecular beam epitaxy with fully compressive strain on a SrRuO3/SrTiO3 substrate. Analysis of the LEED-IV reveals a surface dead layer with a single-domain upward (out of surface) polarized state below. Intrinsic asymmetry and the stability to compensation of depolarizing charges by dipoles induced by surface stress can explain the single domain scenario. Research was sponsored by the Division of Materials Sciences and Engineering and the Center for Nanophase Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC.

3:18PM S37.00005 Phase diagram of Ba0.5Sr0.5TiO3 thin films KRISTOPHER E. ANDERSEN, Northern Arizona University, C. STEPHEN HELLBERG, Naval Research Laboratory — Ba0.5Sr0.5TiO3 (BST) thin films are a promising material for tunable microwave applications, which require large, tunable dielectric constants and low loss. By controlling the (i) substrate and (ii) oxygen partial pressure, it is possible to tune the tetragonal strain of these films. For example, in-plane strains between -0.48% (highly compressive) and +0.30% (highly tensile) have been reported for BST thin films grown on MgO(001) using rf magnetron sputtering. The ability to control the strain makes it possible to optimize the dielectric properties of the film for microwave (and other) applications; however, the strain-temperature phase diagram has not been systematically explored to-date. In this talk, the phase diagram of BST is studied using first-principles calculations, focusing initially on the T = 0 phases. Results for displacive as well as coupled ferroelectric/antiferroelectric phases (recently discussed by Zhang, Cagin, and Goddard in connection to BaTiO3) will be presented.

3:30PM S37.00006 Influence of strain relaxation and atomic interface configuration on the dielectric response of BST thin film capacitors REGINA DITTMANN, RAFAEL PLOKKA, PATRICK SCHÜTZENDORF, PERTSEV NIKOLAY, SHAOBO MI, CHUNLIN JIA, RAINER WASER, Research Centre Juelich — The collapse of the dielectric response which is commonly observed in Ba0.5Sr0.5TiO3 (BST) thin films is a topic of general physical interest as well as a key issue in terms of a possible application of this material in future DRAM storage capacitors. We address the influence of substrates-imposed strain and electrode interface configuration on the dielectric collapse in epitaxial SrRuO3/BST/SrRuO3 thin film capacitors. The growth mode of BST thin films was analyzed by RHEED and HRTEM from the thickness range of a few unit cells up to hundreds of nanometers where plastic strain relaxation occurs. The crystalline quality of our ultrathin samples enabled us to resolve the atomic arrangement and to identify the terminating layers at the SrRuO3/BST interface by STEM. We obtained bulk-like permittivities in the order of 5000 and its thickness dependence can be well described by an extended Ginzburg-Landau-D Devonshire model by taking into account plastic strain relaxation in BST thin films and finite screening of depolarizing fields by the SRO electrodes. We will furthermore present relaxor-type behavior of the BST thin films that becomes visible only in samples with sufficient interface quality and hints on nanoscale structural inhomogeneities.

3:42PM S37.00007 Strain Effects in Barium Strontium Titanate Thin Films for Tunable Microwave Applications LISA ALLDREDGE, WONTAE CHANG, Naval Research Laboratory, JOSEPH WOICIK, National Institute of Standards and Technology, STEVEN KIRCHOFER, JEFFREY POND, Naval Research Laboratory — Recently, it has been demonstrated that control of lattice structure can improve dielectric tuning in epitaxial ferroelectric (FE) films. Understanding the coupling of strain and lattice structure to the dielectric properties is important for FE-based tunable microwave applications. Ba0.5Sr0.5TiO3 films on (001) MgO substrates were grown by sputter deposition with <c> a > and c> a tetragonal distortions, where a and c are the in-plane and out-of-plane lattice parameters, respectively. The dielectric properties were significantly affected by the type of lattice distortion and the interplay of strain and orientation. X-ray absorption near edge structure (XAFS) measurements were taken in several orientations. The anisotropy in the spectra with orientation was used to determine the FE phases of the films. The dependence of the in-plane dielectric constant on strain will be discussed in terms of a theoretical model of the phenomenological thermodynamics of the film strain effect.

3:54PM S37.00008 An ab initio study of strained PZT films SCOTT BECKMAN, KARIN RABE, DAVID VANDER-BILT, Rutgers University — The potential for creating ferroelectric-based devices such as ferroelectric random-access memories (FeRAMs) has led to an intense interest in ferroelectric perovskite thin films, alloys, and superlattices. Engineering of FeRAMs requires the control of both the spontaneous polarization and the barrier for polarization reversal. The two parameters that are simplest to modify are the composition, which is controlled during the film deposition, and the epitaxial strain, which is controlled by substrate selection. Here, using ab initio methods, we investigate how the ferroelectric properties of (PZT) depend upon epitaxial strains ranging from -0.02 ≤ x ≤ +0.02. Compositions ranging from 0.0 ≤ x ≤ 0.5 are examined by the creation of special quasirandom structures. In agreement with the literature, the effect of strain on the polarization is found to be small. We also examine the strain dependence of the barrier for polarization reversal, and discuss the results in the context of experimental measurements of coercive fields and polarization retention.1

4:06PM S37.00009 High pressure x-ray diffraction study of single crystal Pb(Sn0.5 Nb0.5)O3, MADDURY SOMAYAZULU, MUHTAR AHART, RONALD COHEN, Geophysical Laboratory, RUSSELL HEMLEY, Geophysical Laboratory, GEOPHYSICAL LABORATORY TEAM — We employed high pressure single crystal x-ray diffraction to investigate the pressure-induced phase transition in Pb(Sc0.5Sn0.5)O3 (PSN). At 2 GPa and 300 K, PSN undergoes a phase transition as deduced from earlier dielectric measurements. The pressure dependence of diffuse scattering observed around the (110) Bragg peaks indicates that pressure suppresses the local distortion that is coupled to the polar nanoribbons. We have monitored the pressure dependence of diffuse scattering at temperatures between 300 - 4 K and used this to understand the P-T phase diagram of PSN. In addition, we also investigated the equation of state at various temperatures. Observed changes in the isothermal compressibility at low temperatures indicate that the first order phase transition changes character at 200 K and 4 GPa. The results can be understood in terms of a pressure-induced decrease in the correlation length among polar nanoribbons, which is a unique property of relaxor ferroelectrics.

4:18PM S37.00010 Strain induced relaxor behavior in PbSc0.50Nb0.25Ta0.25O3 thin films: A comparison with the nanocrystallites, MARGARITA CORREA, ASHOK KUMAR, RAM KATIYAR, University of Puerto Rico — A comparative study of the microstructure, micro Raman spectroscopy and dielectric properties of PbSc0.50Nb0.25Ta0.25O3 thin films and ceramics were carried out over a wide range of temperature 100-520 K and frequency 100Hz to 1MHz. Microstructure of PSNT films revealed an in-plane compressive strain whereas PSNT ceramics showed an average 10-15 nm size nanoribbons. We observed a shift of 65 K in dielectric maxima temperature towards the lower temperature and frequency dispersion of the dielectric constant in PSNT films compared to bulk that does not exhibit relaxor behavior. We addressed this different dielectric response due to the in-plane compressive strain in the films. Temperature dependent micro Raman spectroscopy revealed that the ferroelectric state in PSNT ceramics were accompanied by pronounced changes in both the lowest frequency F_{2g} and highest frequency A_{1g} modes. Micro Raman spectra of the thin films compared to nanocrystalline showed shifting of the Raman modes to lower frequencies that confirms the strain state of the films. The in-plane compressive strain, dipole arrangement and the size of nanoribbons change the dielectric response of the PSNT films compared to nanocrystallites.

4:30PM S37.00011 First Principles Theory of Sub-Monolayer Strontium on Silicon (001), KEVIN GARRITY, Yale University Department of Physics, JAMES REINER, FREDERICK WALKER, CHARLES AHN, SOHRAB ISMAIL-BEI, Yale University Department of Applied Physics — Conventional attempts to continue transistor scaling consistent with Moore's law will soon result in unacceptable quantum mechanical leakage currents across the dielectric oxide layer. One promising solution to this problem is to replace the current silicon dioxide layer with a thicker crystalline oxide with a higher dielectric constant, grown epitaxially on silicon. Although there has been progress in growing high quality epitaxial interfaces for some materials, the initial stages of growth, including the deposition of the initial metal layer, are not well understood. Using ab initio density functional theory, we study the initial stages of the deposition of strontium titanate on silicon (001), a good model system due its successful epitaxial growth. We present the binding energies of several new low energy structures with sub-monolayer coversages of strontium which differ significantly from the conventional view of this surface. Additionally, to include finite temperature effects, we calculate vibrational free energies. We compare our results to experimental samples grown by molecular beam epitaxy.

4:42PM S37.00012 Sub-monolayer Strontium Phase Diagram on Silicon (100), JAMES REINER, KEVIN GARRITY, FRED WALKER, SOHRAB ISMAIL-BEI, C. H. AHN, Yale University — Crystalline oxides manifest a number of important phenomena, including magnetism, ferroelectricity, superconductivity, and colossal magnetoresistance. Recently, it has become possible to integrate these materials onto a silicon platform in a fully epitaxial structure. These crystalline oxide-silicon heterostructures bring the promise of integrating the rich functionality present in crystalline oxides with modern silicon device technology. The most successful fully epitaxial oxide-silicon (100) heterostructures have been achieved through a deposition recipe that involves manipulating substrate temperature and oxygen pressure on a layer by layer basis during the deposition of an alkaline earth metal. Motivated by a desire to develop a fundamental understanding of this important transition layer between silicon and oxide, we have mapped out the phase diagram of strontium on silicon as a function of temperature and coverage. In particular, recent work on sub-monolayer strontium deposition on the silicon surface suggests the conventional picture of this structure, upon which the entire crystalline oxides on silicon framework is built, is only a low-temperature phase which plays no role in enabling epitaxial oxide growth. Instead, there is strong evidence that a different high temperature phase is the crucial template for epitaxial oxide growth on silicon.

5:06PM S37.00014 Polarization of strained SrTiO3 films grown on Si (001), F. J. WALKER, YARON SEGAL, Yale University, J. W. REINER, C. H. AHN, Yale University, ZHAN ZHANG, Argonne National Laboratory — Perovskite oxides grown on silicon provide powerful new functionalities for device components built upon the ubiquitous silicon platform. A rich set of applications results from the combination of the perovskite’s diverse electrical and physical structures and the semiconducting properties of silicon. Understanding how to develop new functionalities, however, requires detailed knowledge of the real space positions of atoms with sub-angstrom resolution. In this work, we have carried out synchrotron x-ray diffraction studies of crystal truncation rods on 4-5 unit-cell-thick SrTiO3 films grown epitaxially on silicon, which have been terminated with different gate materials. We determine the precise atomic structure of these materials, in particular the displacements of the TiO2 planes relative to the SrO planes that make up the perovskite structure. We show how that the polarization and structure of commensurately strained films depend critically upon the electrical and chemical properties of the terminating metal.

5:18PM S37.00015 Writing and Reading of Ultrathin Ferroelectric Domains on Commensurate SrTiO3 on Silicon, JEREMY LEVY, YUN JIN PARK, JEREMY LEVY, KYUNGJIN LEE, KUSHAL SRIVASTAVA, JEREMY LEVY, CHENG CEN, CHARLES R. SLEASMAN, MAITRI WARUSAWITHANA, DARRELL G. SCHLOM — Ferroelectricity in ultrathin epitaxial SrTiO3 grown commensurately by oxide-molecular beam epitaxy (MBE) on silicon substrates was investigated using piezoresponse force microscopy (PFM). A series of samples containing n multilayers (ML) of SrTiO3 (n = 3, 4, 5, 6, 8, 10, 20) was grown on silicon substrates. Room-temperature ferroelectricity was observed for all samples containing n = 5, 6, 8, 10 ML. Temperature-dependent measurements indicate that the sample with n = 5 exhibits a ferroelectric phase transition at T_C = 317 K. Sample with n = 6 remains ferroelectric up to at least 393K. Polar domains created on the n = 6 was found to be stable at room temperature for more than 72 hours. The implications of these results for fundamental and device-related applications will be discussed briefly.

This work was supported by NSF-0704022 (JL) and Office of Naval Research (ONR) through grants N00014-03-1-0721 (DGS) and N00014-04-1-0426 (DGS) monitored by Colm Wood.
2:30PM S39.00001 Absorbing-state phase transitions: exact solutions of small systems. RONALD DICKMAN, UFMG — I derive precise results for absorbing-state phase transitions using exact (numerically determined) quasistationary (QS) probability distributions for small systems. Analysis of the contact process on rings of 23 or fewer sites yields critical properties (control parameter, order-parameter ratios, and critical exponents $\alpha$ and $\beta/\nu$) with an accuracy of better than 0.1%; for the exponent $\nu$, the accuracy is about 0.5%. Good results are also obtained for the pair contact process. The QS kurtosis exhibits a sharp minimum at the critical point.

$^1$This work was supported by CNPq and FAPEMIG, Brazil.

2:42PM S39.00002 Displacement and velocity correlation functions of magnetic particle chains undergoing Brownian dynamics. YUK KWAN HO, MINGJIE ZHENG, KIN WAH YU, The Chinese University of Hong Kong — Brownian dynamics of physical systems has been studied for a long time since Einstein in 1905. In this work, we report the study of a magnetic particle chain in ferrofluid, with hydrodynamic interactions and harmonic interactions included, by using Rice method [1]. We will focus on the correlation functions and relaxation time of the chain. As qualitative account for the effect of system parameters, analytic solutions of the displacement and velocity correlation functions of a two-body system have been studied. In the case of an over-damped system, very long relaxation time for the displacement correlation function can be obtained from the analytic solutions. Moreover, the size dependence of the relaxation time is also studied numerically for moderate chain sizes.


2:54PM S39.00003 Theory of Zener tunneling and breakdown in solids. NAOYUKI SUGIMOTO, Department of Applied Physics, University of Tokyo, SHIGEKI ONODA, RIKEN, NAOITO NAGAOASA, Department of Applied Physics, University of Tokyo, CERC, CREST — Tunneling and breakdown phenomena are among of the most important problems in condensed matter physics. We study the Zener tunneling and breakdown phenomena in a bulk system taking into account the dissipation due to impurity scatterings in terms of the Keldysh formalism. Three distinct regions are recognized for the current-field characteristics, which are identified as the impurity-conduction, the Zener tunneling, and the Zener breakdown, respectively. The crossovers among them are described in a unified fashion. By examining the local density of states, which can be measured by scanning tunneling spectroscopy, we find that the Zener tunneling and breakdown can be understood as the conductance due to the finite local density of states at the Fermi energy originating from the hybridization between the conduction and valence bands induced by the electric field.

3:06PM S39.00004 Domain Structure Universality in Coarsening. BENJAMIN VOLLMAYR-LEE, Bucknell University, ANDREW RUTENBERG, Dalhousie University, SOHEI YASUDA, Bucknell University — Coarsening systems ubiquitously exhibit power law growth $L \sim t^{\alpha}$ with self-similar domain morphology, and much progress has been made in mapping out universality classes of the growth exponent $\alpha$. It has been commonly argued that these universality classes should apply well to the scaled domain structure, but recent evidence has appeared to the contrary. In particular, surface tension anisotropy has been found numerically and by exact solutions in the dilute limit to modify the domain morphology and structure factor, while leaving growth exponents unchanged. Thus the universality classes of the domain morphology remains an open question. We present a conjecture that the morphology universality is a consequence of the asymptotic trajectories of the topological defects, and then map out the universality classes that follow. Our prediction, in the case of scalar, conserved order parameter coarsening, is that the domain structures depend on surface tension anisotropy and mobility asymmetry, but nothing more. To test this prediction we have conducted extensive simulations of coarsening with mobility asymmetry and have demonstrated its influence on the scaled domain structure.

3:18PM S39.00005 Exact Solutions for Anisotropic Coarsening in the Dilute Limit. WILLIAM ROSENBAUM, Reed College, MELINDA GILDNER, BENJAMIN VOLLMAYR-LEE, Bucknell University — We study the influence of anisotropy on coarsening dynamics via two dilute coarsening models: Lifshitz-Slyozov theory for locally conserved order parameter dynamics, and Wagner theory for the globally conserved analog. We adopt a perturbative approach to analyze the effect of surface tension anisotropy on drop shapes and the scaled drop size distribution. In both models we find that coarsening solutions exhibit growth laws that are unchanged from the isotropic theories, $L \sim t^{1/3}$ and $L \sim t^{1/2}$ respectively, and drop shapes that are in general nonspherical and non-Wulffian. We also determine that the drop size distribution varies from the isotropic case.

3:30PM S39.00006 Domain Morphology and Structure Factor in the Asymmetric Cahn-Hilliard equation. SOHEI YASUDA, BENJAMIN VOLLMAYR-LEE, Bucknell University, ANDREW RUTENBERG, Dalhousie University — The Cahn-Hilliard equation for conserved order parameter coarsening is modified to allow for unequal mobilities in the two equilibrium phases. This asymmetric Cahn-Hilliard equation is then simulated using an unconditionally stable algorithm, which enables reaching times well into the $L \sim t^{1/3}$ dynamic scaling regime. Our goal is to address questions of the universality of the scaled domain morphology; in particular, to test our conjecture that the morphology should depend on the mobility asymmetry. We study mobility ratios of 1, 2, 4 and 8 and find that the domain size distribution depends strongly on the mobility asymmetry: the higher (lower) mobility phase forms a smaller (larger) backbone cluster with more (fewer) smaller domains, and the magnitude of the effect grows with the mobility ratio. Interestingly, the structure factor shows no discernible dependence on the mobility asymmetry.

3:42PM S39.00007 Non-trivial statistics crossover in random sequential adsorption due to the presence of a pattern. NUNO A.M. ARAUJO, GCEP-Centro de Física da Universidade do Minho, 4710 Braga, Portugal; T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ANTONIO CADILHE, T-12 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; GCEP-Centro de Física da Universidade do Minho, 4710 Braga, Portugal, VLADIMIR PRIVMAN, Department of Physics, and Center for Advanced Materials Processing, Clarkson University, Potsdam, NY 13699, USA — The random sequential adsorption (RSA) on a lattice approaches the jammed state exponentially, while in the off-lattice version approaches the jammed state as a power-law. In this presentation, we focus on the kinetics leading to the jammed state. The presence of pattern influences the kinetics of approach to the jammed state. Namely, a pattern consisting of equal size squares embedded on a square matrix lattice provides a rich set of regimes. Measurements of the distribution of areas available for adsorption during the process make possible to predict how the jammed state is attained: power-law or exponential. Finally, we associate these two different kinetic regimes with the breakdown of Pommeau statistics near the jammed state.
apparently cannot be rigorously derived by any existing technique. The checkerboard formula that we find is same as that conjectured by Wu (Rev. Mod. Phys.

Increasingly accurate approximations. For the Archimedean lattices the critical thresholds we find by this method are accurate to at least 4 significant figures.

Critical surfaces for general two dimensional lattices. Our approach is to assume that the critical surface is at most first order in its arguments and then to

The multifractal exponents of the fractal surfaces. For DLA, we address the controversy of the behavior of the harmonic measure deep inside the fjord.

Linear in the number of sites considered. The method works for lattice systems and discretized versions of continuum systems. With it, we have solved for

Solves for those measures is developed. The technique uses a step-by-step approach that adds a shell at each time step to the diffusion front, and is essentially

fjords and inlets of irregular surfaces, traditional methods of solving Laplace's equation become very inefficient. A new numerical algorithm that efficiently

A new numerical algorithm that efficiently

3:54PM S39.00008 Dephasing and the steady state in quantum many-particle systems. THOMAS BARTHUL, ULRICH SCHOLLWÖCK, Institute for Theoretical Physics C, RWTH Aachen, Germany — We discuss relaxation in many-particle systems. For integrable systems, the time-evolution from an arbitrary initial state can lead, for a given finite subsystem, to a definite steady state. We give an explicit derivation of the steady state ensemble and devise sufficient prerequisites for the dephasing to take place. We also find surprisingly simple scenarios, in which dephasing is ineffective and discuss the dependence on dimensionality and criticality. It also follows that, after a quench of system parameters, entanglement entropy will become extensive.

1 T. B. thanks the DFG for support.

4:06PM S39.00009 Assembly and control of self-propelled structures in driven suspensions of magnetic microparticles. MAXIM BELKIN, Illinois Institute of Technology / Argonne National Lab, ALEXEY SNEZHKO, IGOR ARANSON, WAI-KWONG KWOK, Argonne National Lab — Magnetic microparticles suspended on the surface of liquid and subjected to periodic vertical magnetic excitations form a non-trivial dynamic snake-like pattern accompanied by large-scale surface flows. Apparently, controlled suppression of vortices at one end of the snake may lead to a formation of a self-propelled structure. We demonstrate that the suppression of the vortex pair can be implemented by the mechanical disturbance of the one end of the structure by means of the floating particle with characteristic size comparable to the width of the snake’s segment. The snake structure with the particle attached to its end becomes a swimmer with parameters effectively controlled by the external driving magnetic field. Experimental studies of such self-propelled structures are presented.

4:18PM S39.00010 Avalanches of Bose-Einstein-Condensates from open optical lattices. TSAMIKOS KOTTOS, Department of Physics, Wesleyan University, Connecticut-USA and MPI for Dynamics and Self-Organization, Gottingen-Germany, GIM SENG NG, Department of Physics, Wesleyan University, Connecticut-USA, HOLGER HENNIG, RAGNAR FLEISCHMANN, THEO GEISEL, MPI for Dynamics and Self-Organization, Gottingen-Germany — We investigate, the outgoing atomic flux of BECs loaded in large OLs using a mean field (Discrete Non-Linear Schroedinger Equation—DNLSE) approach. We show that for some critical values of the rescaled (with respect to the lattice size) interatomic interaction strength, the current decays in avalanches that follow a power-law distribution indicating the existence of a novel phase transition. The origin of this phenomenon is identified to be the collisions between stable and moving breathers which co-exist at the lattice. Using a reduce map we are able to provide bounds for the power law exponent of the avalanche distribution which reflect the complexity of the underlying classical phase-space. Due to the inter-disciplinary nature of the DNLS, we expect that the same phenomenon will be observed in several other branches of nonlinear physics, ranging from nonlinear optics to polaron and biological molecules.

3USA-Israel Binational Science Foundation and DFG (KO 3608/1-1)

4:30PM S39.00011 Study of universality and critical behavior in periodically driven interacting cold atomic system. MYOUNG-SUN HEO, YONGHEE KIM, WONHO JHE, Seoul National University, HEUNG-RYOL NOH, Chonnam National University — Strongly driven nonlinear oscillators show a variety of interesting phenomena such as period doubling, bifurcation, chaos. Since their resonant behaviors are very sensitive to external perturbation, they have now been widely adopted for the precise determination of physical quantities. The key concept to these researches is the development of bistable or period-2 states, which are, in most cases, energetically degenerate. If particles interact each other, however, this degeneracy of two attractors can be lifted up. For example, in the simple case of all-to-all attractive interaction, particles will be preferably directed into more populated attractors. Being incorporated with random fluctuation which tries to equilibrate population in each attractor, this lifting-up becomes dependent on the system size, or the total number of particles, as recently observed as spontaneous symmetry breaking in cold atomic system which inherently possesses the light-induced attractive interaction. In particular, this dependence seems to show a sort of critical behavior. Here we have elucidated the criticality existing in the strongly driven interacting many-particle system consisted up of cold atoms from static and dynamic perspectives.

4:42PM S39.00012 Transition of Electromechanical Pendulum into Nonlinear Response. CHULKI KIM, Physics, University of Wisconsin-Madison, HUA QIN, HYUN-SEOK KIM, ROBERT BLICK, Electrical & Computer Engineering, University of Wisconsin-Madison — We present measurements on a macroscopic electron shuttle in the regime of nonlinear response. The shuttle is formed by a classical mechanical pendulum situated between two capacitor plates. The main advantage of this macroscopic setup is that we can directly measure the onset of nonlinear response of thiselectromechanical pendulum exhibiting period doubling. The results will find use in application such as bifurcation amplifier in nanoscopic versions of the device. A model nanoelectromechanical device based on the macroscopic experiment has the potential to reveal nonlinear quantum mechanical effects.

4:54PM S39.00013 Harmonic measure of DLA and percolation clusters. ROBERT ZIFF, LEONARD SANDER, DAVID ADAMS, University of Michigan — The problem of efficiently finding the harmonic measure of DLA and percolation clusters is addressed. Deep inside fjords and inlets of irregular surfaces, traditional methods of solving Laplace’s equation become very inefficient. A new numerical algorithm that efficiently solves for those measures is developed. The technique uses a step-by-step approach that adds a shell at each time step to the diffusion front, and is essentially linear in the number of sites considered. The method works for lattice systems and discretized versions of continuum systems. With it, we have solved for the multifractal exponents of the fractal surfaces. For DLA, we address the controversy of the behavior of the harmonic measure deep inside the fjord. For percolation, we consider both the relatively smooth accessible hull (D = 4/3), and the very invaginated regular hull (D = 7/4).

5:06PM S39.00014 Critical surfaces for general two dimensional bond percolation problems. CHRIS SCULLARD, University of Chicago, ROBERT ZIFF, University of Michigan — We present a general method for deriving approximate bond percolation critical surfaces for general two dimensional lattices. Our approach is to assume that the critical surface is at most first order in its arguments and then to impose symmetries and known special cases until the function is completely determined. We show also that allowing higher powers of the arguments gives increasingly accurate approximations. For the Archimedean lattices the critical thresholds we find by this method are accurate to at least 4 significant figures. In two other cases, the checkerboard and inhomogeneous bow-tie we find critical surfaces that appear, from our numerical investigation, to be exact but that apparently cannot be rigorously derived by any existing technique. The checkerboard formula that we find is same as that conjectured by Wu (Rev. Mod. Phys. 54, 235 – 265 (1982)).
5:18PM S39.00015 Nonuniversal Deviations From Predictions of the Random Matrix Theory of Wave Chaotic Scattering: Theory and Experiment1. STEVEN ANLAGE, JAMES HART, ELLIOTT BRADSHAW, THOMAS ANTONSEN, EDWARD OTT, Physics Department, University of Maryland — The eigenfunctions and spectra of chaotic billiards are notoriously sensitive to small perturbations. Thus statistical approaches have been developed to model such systems. In recent work, we used random matrix theory to develop statistical models for the impedance of a chaotic microwave cavity coupled to a small number of antennas, with the only parameters being the radiation impedance of the antennas, the area of the cavity and a uniform loss parameter Q [S. Hemmady, et al., Phys. Rev. Lett. 94, 014102 (2005); X. Zheng, et al., Electromagnetics 26, 3 (2006)]. The theory generally agrees well with experiment, but under some circumstances the experimental and numerical results deviate significantly from the Random Matrix Theory predictions. We have derived a method of accounting for these deviations and have experimental and numerical results which agree well with our new, non-universal, predictions.

1Work supported by ONR MURI and AFOSR.

Wednesday, March 12, 2008 2:30PM - 4:06PM –
Session S40 FHP: History of Physics Morial Convention Center 232

2:30PM S40.00001 Development of ultra violet photoemission [UPS]: a history1, JERRY [G. J.] LAPEyre — UPS of solids investigations are summarized from the late 1940’s through the very early 1960’s which measured kinetic energy distributions [EDC’s] of the emitted electrons. The experiments contributed to the opening of the photoemission spectroscopy fields. This era involved activities at G. E. Research Labs, Univ. of Missouri and W. E. Spicer’s lab. The author knew most of the researchers.

1DoE, ONR, NSF

2:54PM S40.00002 Magnetism in matter before the discovery of quantum spin: Bohr’s less well-known contribution to the transition from classical to quantum physics. JEAN-FRANCOIS VAN HUELLE, Brigham Young University — How does one explain magnetic effects in matter when one views matter as a collection of classical charges in motion? The answer is: not at all! This is one of the points that Niels Bohr made in his doctoral dissertation in 1911, two years before addressing the issue of the stability of the hydrogen atom. The result, later rediscovered by H.J.van Leeuwen was amplified and formalized in Van Vleck’s 1932 text on electric and magnetic susceptibilities and it is currently known as the Bohr-van Leeuwen theorem. We will review Bohr’s two derivations, one statistical and one based on the motion of individual electrons. We will then propose reasons why this result, unlike that on the stability of hydrogen, did not lead to a major development in quantum theory but, instead, had to wait until after the introduction of spin and exchange forces in quantum mechanics to become generally known.

3:18PM S40.00003 Epistemological Dimensions in Niels Bohr’s Conceptualization of Complementarity, GREGORY DERRY, Loyola College In Maryland — Contemporary explications of quantum theory are uniformly ahistorical in their accounts of complementarity. Such accounts typically present complementarity as a physical principle that prohibits simultaneous measurements of certain dynamical quantities or behaviors, attributing this principle to Niels Bohr. This conceptualization of complementarity, however, is virtually devoid of content and is only marginally related to Bohr’s actual writing on the topic. Instead, what Bohr presented was a subtle and complex epistemological argument in which complementarity is a shorthand way to refer to an inclusive framework for the logical analysis of ideas. The important point to notice, historically, is that Bohr’s work involving complementarity is not intended to be an improvement or addition to a particular physical theory (quantum mechanics), which Bohr regarded as already complete. Bohr’s work involving complementarity is actually an argument related to the goals, meaning, and limitations of physical theory itself, grounded in deep epistemological considerations stemming from the fundamental discontinuity of nature on a microscopic scale.

3:42PM S40.00004 Paradox, Natural Mathematics, Relativity and Twentieth-Century Ideas, JOHN RYSKAMP — We are enjoying a renaissance in the historiography of set theory which allows us to pinpoint the effect of Poincare’s writing on the development of Einstein as an advocate of natural mathematics (what he called practical geometry). I will briefly describe the importance of Garciadiego’s landmark work on Russell (1992), and Grattan-Guinness’ epic recounting of the history of set theory (2000). I will present something for which historians of physics have searched but have not previously identified: the precise step at which Einstein incorporated practical geometry into his formulation of the relativitity of simultaneity. This leads to a troubling conclusion, at least for those who look to relativity for internal consistency. However, the trouble is not restricted to physics. We suggest that natural mathematics finds its way into the major twentieth-century ideas.

Wednesday, March 12, 2008 7:30PM - 9:00PM –
Session T1 Quarks to Cosmos: Breaking News at the Interface of Particle, Nuclear and Astrophysics New Orleans Marriott Carondelet (3rd floor)

7:30PM T1.00001 Quarks to Cosmos: Breaking News at the Interface of Particle, Nuclear and Astrophysics, MICHAEL TURNER, University of Chicago, JOSEPH LYKKEN, Fermi National Accelerator Laboratory, MICHAEL WIESCHER, University of Notre Dame — Profound connections join scales all the way from the very smallest to the very largest that we can explore, and these connections now link the fields of astrophysics, cosmology, nuclear physics and particle physics. Research that crosses these traditional field boundaries are beginning to reveal new states of matter, how the Universe began, the role of neutrinos in shaping the Universe, how massive stars explode and the elements in the periodic table were made, how Nature’s most powerful accelerators work, the nature of space and time and the unification of the forces, and the nature of dark matter and dark energy. These three talks will showcase these connections, highlight recent exciting results, and look toward the future.

Wednesday, March 12, 2008 5:30PM - 7:05PM –
Session T16 GSCCM: Town Hall Meeting: Materials Physics at Gigabar Pressures Morial Convention Center 208

5:30PM T16.00001 Introduction —
energy between the singlet and triplet lowest states of substantial, and as important as the electron phonon interaction. This leads to relatively large intrachain exciton binding energy of ∼0.7 eV. (ii) There are few important excited states with odd and even parity symmetry that govern the optical, electrical and magnetic properties of these materials; including electron-phonon interaction, electron-electron (e-e) and electron-hole (e-h) interactions, interchain coupling, spin-lattice and spin-orbit coupling. These properties are very important for various optoelectronic applications, in which the polymers serve as active layers. The following picture of the excited state properties of these polymers has emerged. (i) The e-e and e-h interactions are crucial part of this understanding is the properties of materials under extreme conditions. Typical conditions inside Jupiter are megabars and ten thousand kelvin, accessible in lab experiment and through simulation. Typical materials are cosubstantially abundant hydrogen, helium, oxygen, carbon and nitrogen (in appropriate mixtures) and also Earthlike ("rock" and iron). Equation of state, including slopes of isentropes, etc, phase diagrams and transport properties (especially electrical conductivity) are of particular interest. I will describe some of the outstanding unsolved problems for planets, including extrasolar planets more massive than Jupiter.

6:35PM T16.00004 Physics of matter at extreme densities, theoretical perspectives, RICHARD MARTIN, — This abstract not available.

Thursday, March 13, 2008 8:00AM - 11:00AM
Session U1 DCMP DMP: Isakson Prize, Adler Award, Nicholson Medal Session
Morial Convention Center LaLouisiane AB

8:00AM U1.00001 TBD, MITCHELL FEIGENBAUM, Rockefeller University — No abstract available.

8:36AM U1.00002 Frank Isakson Prize Talk: Using ultrafast to probe the slow1, JOSEPH ORENSTEIN, UC Berkeley and LBNL — The field of ultrafast optics exploded on the scene with the development of mode-locked lasers, and continues to grow as technology evolves. Although often associated with highly-nonequilibrium phenomena, ultrafast experiments can be performed in a low-power regime in which electronic systems are tickled, rather than blasted. The amplitude and phase stability of today’s laser oscillators allows detection of very small changes in optical response that result from weak laser excitation. While these changes can be viewed as a form of linear response, they often reveal properties that are not detected by traditional probes such as electrical conductivity or magnetic susceptibility. In this talk I will describe two examples of this approach, in the fields of high-Tc superconductivity and spin propagation in semiconductors. Somewhat paradoxically, the use of ultrafast techniques allows the observation of some rather slow effects. In the high-Tc materials, the lifetime of the photoexcited state diverges as the optical energy per laser pulse is lowered. The slow dynamics in this regime provide a window to the intrinsic inelastic scattering rate of quasiparticles, a new collective mode, and an abrupt transition in dynamics that takes place as a function of doping. In GaAs quantum wells the stability of the laser oscillator enables phase-sensitive detection of a transient spin-polarization wave that result from weak laser excitation. While these changes can be viewed as a form of linear response, they often reveal properties that are not detected by traditional probes such as electrical conductivity or magnetic susceptibility. In this talk I will describe two examples of this approach, in the fields of high-Tc superconductivity and spin propagation in semiconductors. Somewhat paradoxically, the use of ultrafast techniques allows the observation of some rather slow effects. In the high-Tc materials, the lifetime of the photoexcited state diverges as the optical energy per laser pulse is lowered. The slow dynamics in this regime provide a window to the intrinsic inelastic scattering rate of quasiparticles, a new collective mode, and an abrupt transition in dynamics that takes place as a function of doping. In GaAs quantum wells the stability of the laser oscillator enables phase-sensitive detection of a transient spin-polarization wave generated by the interference of two excitation pulses. Measuring dynamics as function of wave vector fully characterizes the spin propagation, revealing effects such as ballistic to diffusive crossover and spin Coulomb drag. In these systems we again have focused on “slow” phenomena. I will describe some of our recent attempts to create and detect a long-lived, “persistent spin-helix” state, predicted to occur at special points in the spin-orbit coupling parameter space.

1Research supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, DOE.

9:12AM U1.00003 Frank Isakson Prize Talk: Optical Probes of π-Conjugated Polymers1, Z. VALY VARDENY, University of Utah — We review several optical probes that have been applied to π-conjugated polymers over a time period of ~30 years. These include linear and nonlinear optical spectroscopies, resonant Raman scattering, transient and steady state photodynamics, photoinduced electron and hole action, and optically detected magnetic resonance spectroscopy. The application of these techniques has revealed a myriad of important information on the interaction that govern the optical, electrical and magnetic properties of these materials; including electron-phonon interaction, electron-electron (e-e) and electron-hole (e-h) interactions, interchain coupling, spin-lattice and spin-orbit coupling. These properties are very important for various optoelectronic applications, in which the polymers serve as active layers. The following picture of the excited state properties of these polymers has emerged. (i) The e-e and e-h interactions are substantial, and as important as the electron phonon interaction. This leads to relatively large intrachain exciton binding energy of ~0.5 eV, and exchange energy between the singlet and triplet lowest states of ~0.7 eV. (ii) There are few important excited states with odd and even parity symmetry that govern the nonlinear optical spectra of these materials. (iii) The primary photoexcitations are intrachain excitons in isolated chains, and both excitons and polaron pairs in chains coupled by interchain interaction. (iv) The most strongly coupled phonons are amplitude modes of which frequencies and oscillator strengths are very sensitive to the existence of excess charges on the chains. (v) Excite changes are accommodated on the chains in the form of polarons with relatively large relaxation energy ranging from 0.1 to 0.5 eV. (vi) The spin orbit coupling is very weak in these materials, but can be tuned by involving heavy atoms in the polymer building blocks. (vii) The spin relaxation time for spin 1/2 polarons is relatively long of ~1 microsecond. The two latter properties may lead to new applications in the field of Organic Spintronics.

1Supported by the DOE and NSF-DMR.

9:48AM U1.00004 David Adler Lectureship Award Talk: Lattice instabilities and ferroelectricity in complex oxides, KARIN M. RABE, Rutgers University — In perovskite oxides, layered perovskites and other complex-structured oxide families, a wide variety of distorted equilibrium structures can be realized, including ferroelectric, antiferroelectric, antiferrodistortive, and mixed-character structures. For an individual material, the equilibrium structure can be understood as being produced by the freezing-in of one or more lattice instabilities of the high-symmetry reference structure. This concept is central to the long-established soft-mode theory of ferroelectricity. In fact, first-principles phonon-dispersion calculations show that the high-symmetry reference structures of many complex oxides have entire ranges of instabilities that do not contribute to the bulk ground state structure. In this talk, we discuss how the information from first-principles studies of these systems provides guidance for altering the balance of the competition of instabilities of different character through changes in electrical and mechanical boundary conditions characteristic of epitaxial thin films, superlattices, and nanoparticles, leading to the realization of non-bulk phases. For example, it has been shown both theoretically and experimentally that SrTiO3, which has a nonpolar bulk ground state, can be driven ferroelectric by epitaxial strain. To illustrate the further development and application of these ideas, we present results for CaTiO3 and discuss other materials which, while nonpolar in bulk, can be driven in this way through a phase boundary to become ferroelectric. New ferroelectrics thus obtained could have combinations of tunable properties, including switchable polarization, magnetic ordering, and dielectric and piezoelectric response, desirable for current and future technological applications.
superconducting states, and its relation to the similar SO(4) invariance between the d-density wave and d-wave superconducting states.

via the electronic nematic order and its domains. I will also discuss an SO(4) invariance at the critical point between the electronic nematic and d-wave

consecutive metamagnetic transitions, a large residual resistivity, and an anisotropic magnetoresistance observed in the bilayer ruthenate can be understood

with the discovery of anisotropic quantum Hall phases in GaAs-heterostructures in large magnetic fields. A series of recent experiments on the bilayer ruthenate

that the electronic nematic phase with a broken rotational symmetry is a generic ground state of a doped Mott insulator, and it has attracted much attention

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hole-doped region grows below ~150 K with decreasing temperature, similar to the case in 2DEGs, albeit the much higher temperature scale. In those

samples, the easy transport axis was apparently dictated by the orthorhombic crystal structure; however, the orthorhombicity η was only up to 1.5%, while the resistivity anisotropy was up to a factor of 3, which was obviously too large for the small η. Furthermore, the anisotropy in YBCO was found to be enhanced with decreasing y below ~0.5 despite the decreasing η until the crystal structure turns to tetragonal at y = 6.30. While this result gave strong evidence for the self-organization of the EN in high-Tc superconductors, it was not completely conclusive because of the existence of the orthorhombicity that chooses the preferred direction; also, the lack of support from neutron scattering kept the skepticism remain. However, very recently, neutron scattering has finally found corroborating

anisotropy in YBCO and convincing evidence for EN in a related oxide Sr3Ru2O7 was obtained, which together strengthened the case for cuprates considerably.

In collaboration with Kouji Segawa, Seiki Komiya, and A. N. Lavrov.

1Support has been provided by the National Science Foundation

Thursday, March 13, 2008 8:00AM - 11:00AM —

Session U2 DCMP: Electron Nematics

Morial Convention Center LaLouisiane C

8:00AM U2.00001 Transport anisotropy as a signature of electron nematicity

YOICHI ANDO,

Institute of Scientific and Industrial Research, Osaka University — Strong electron correlations often give rise to novel phenomena that are never found in ordinary materials. One of such phenomena is the emergence of electron nematicity (EN), which was theoretically proposed in 1998 to occur due to a combined effect of electron self-organization and quantum fluctuations. Experimentally, the EN was first discovered in 1999 in the two-dimensional electron gas (2DEG) at high Landau levels, where a clear transport anisotropy was found to grow upon lowering temperature in the mK region. In search for the signatures of the EN in cuprates, we have done extensive transport measurements of La2−xSrxCuO4 (LSCO) and YBa2Cu3O7 (YBCO) systems using high-quality single crystals. We discovered in 2001 that the in-plane resistivity anisotropy in untwinned single crystals of LSCO and YBCO in the lightly hole-doped region grows below ~150 K with decreasing temperature, similar to the case in 2DEGs, albeit the much higher temperature scale. In those samples, the easy transport axis was apparently dictated by the orthorhombic crystal structure; however, the orthorhombicity η was only up to 1.5%, while the resistivity anisotropy was up to a factor of 3, which was obviously too large for the small η. Further...

8:36AM U2.00002 Theory of the nematic quantum critical point in a nodal superconductor

EUN-AH KIM, Stanford University — In the last several years, experimental evidence has accumulated in a variety of highly correlated electronic systems of new quantum phases which (for purely electronic reasons) spontaneously break the rotational (point group) symmetry of the underlying crystal. Such electron "nematic" phases have been seen in quantum Hall systems[1], in the metamagnetic metal Sr3Ru2O7[2], and more recently in magnetic neutron scattering studies of the high temperature superconductor, YBCO[3]. In the case of a high Tc superconductor, the quantum dynamics of nematic order parameter naturally couples strongly to quasiparticle (qp) excitations. In this talk, I will discuss our recent results on the effects of the coupling between quantum critical nematic fluctuations and the nodal qp's of a d-wave superconductor in the vicinity of a putative quantum critical point inside the superconducting phase. We solve a model system with N flavors of quasiparticles in the large N limit[4]. To leading order in 1/N, quantum fluctuations enhance the dispersion anisotropy of the nodal excitations, and cause strong scattering which critically broadens the quasiparticle peaks in the spectral function, except in the vicinity of the NWissenstein, L.N. Pfeiffer, and K.W. West, PRL 83, 824 (1999).

1M. P. Lilly, K.B. Cooper, J.P. Eisenstein, L.N. Pfeiffer, and K.W. West, PRL 83, 824 (1999).


3Stanford Institute for Theoretical Physics

9:12AM U2.00003 Metamagnetic Nematic Phase of Sr3Ru2O7, ANDREW MACKENZIE, University of St Andrews — In this talk I will review our group's recent observations that a quantum phase with pronounced electrical transport anisotropies forms in the vicinity of a metamagnetic quantum critical point in Sr3Ru2O7. The behaviour, which is strongly dependent on disorder and is only seen in the highest purity crystals, has phenomenological similarities with prior observations on two-dimensional electron gases in semiconductor devices [1, 2]. Its appearance in bulk in Sr3Ru2O7 has allowed us to perform a number of thermodynamic measurements, and also offers the promise of study using modern surface-based spectroscopies such as angle resolved photoemission and spectroscopic imaging scanning tunneling microscopy. References [1] For example M.P. Lilly et al., Phys. Rev. Lett. 82, 394 (1999); ibid 83, 824 (1999) [2] W. Pan et al., Phys. Rev. Lett. 83, 820 (1999). Collaborators: S.A. Grigera1, R.A. Borzi2, A. Rost1, J.F. Mercure1, J. Farrell1, R.S. Perry2, A.G. Green3, M. Allan3, M. Wang3, J. Lee3, F. Baumberger1, S.J.S. Lister4, S.L. Lee4, J.C.S. Davis5, Z.X. Shen6, Y. Maeno6, 1University of St Andrews, Scotland 2INTA, La Plata, Argentina 3University of Edinburgh, Scotland 4Cornell University, USA 5Stanford University, USA 6Kyoto University, Japan.

9:48AM U2.00004 Electronic Nematic Liquid in Correlated Systems, HAE-YOUNG KEE — It was proposed that the electronic nematic phase with a broken rotational symmetry is a generic ground state of a doped Mott insulator, and it has attracted much attention with the discovery of anisotropic quantum Hall phases in GaAs-heterostructures in large magnetic fields. A series of recent experiments on the bilayer ruthenate Sr3Ru2O7 also suggest the existence of an anisotropic metallic phase which is uncovered by tuning the magnetic field. In this talk, I will show that two consecutive metamagnetic transitions, a large residual resistivity, and an anisotropic magnetoresistance observed in the bilayer ruthenate can be understood via the electronic nematic order and its domains. I will also discuss an SO(4) invariance at the critical point between the electronic nematic and d-wave superconducting states, and its relation to the similar SO(4) invariance between the d-density wave and d-wave superconducting states.

1NSERC of Canada, Canadian Institute for Advanced Research, Canada Research Chair
10:24AM U2.00005 Spins in cuprates near the edge of the superconducting phase - incoherent pairing, fluctuations on all timescales and observation of pseudogap energies. BILL BUYERS, National Research Council, Chalk River — When doping is just enough to create the superconducting phase spins behave very differently from heavily doped cuprates. Nonetheless low doping reveals the key ingredients for the coherence of superconducting pairs. The ordered spins of the insulating antiferromagnet are replaced by a hedgehog phase with isotropically polarized spins, and a commensurate central mode with slow short-range spin correlations extending over four planar unit cells. A subcritical 3D enhancement is destroyed by temperature and energy. The spins follow not via the coherence of charge pairs but the structures caused by hole doping, so that glassy short range spin orders within both the superconducting and normal phase. The tumbling regions of spins exhibit a power-law spectrum similar to 1/f noise down to microeV energies. Excitations are overdamped with a milliEV relaxation rate a thousand times faster, unlike the well-defined resonance familiar at large doping. Below 50 K the scale length is geometric and not linked by velocity to dynamic widths. As excited states are depopulated spin weight transfers to the central mode. At energies 300,000 times larger, decay of paramagnons into pseudogap states has been detected [1], a strong indication that it is the large density of high-energy spin states that provides the superconducting glue, rather than the resonance which is absent as a sharp spectral feature.


Thursday, March 13, 2008 8:00AM - 11:00AM –
Session U3 DPOLY: Simple Views on Polymers at Surfaces and Interfaces: Symposium Honoring P G de Gennes 
Morial Convention Center R02 - R03

8:00AM U3.00001 Polymer adsorption , JEAN-FRANCOIS JOANNY, Institut Curie Paris France — The aim of this talk is to review Pierre-Gilles deGennes’ work on polymer adsorption and the impact that it has now in our understanding of this problem. We will first present the self-consistent mean-field theory and its applications to adsorption and depletion. De Gennes most important contribution is probably the derivation of the self-similar power law density profile for adsorbed polymer layers that we will present next, emphasizing the differences between the tail sections and the loop sections of the adsorbed polymers. We will then discuss the kinetics of polymer adsorption and the penetration of a new polymer chain in an adsorbed layer that DeGennes described very elegantly in analogy with a quantum tunneling problem. Finally, we will discuss the role of polymer adsorption for colloid stabilization.

8:36AM U3.00002 Polymer brushes , EKATERINA ZHULINA, Institute of Macromolecular Compounds, Russia — The polymer brush is an ensemble of macromolecules end-tethered to a substrate. The so-called Alexander-de Gennes polymer brush model (S. Alexander, J. Physique 1977, and P.-G. de Gennes, Macromolecules 1980) opened a new field in polymer science and provided a theoretical framework to look at brush-like polymer systems. In this presentation, we will first briefly review the ideas and concepts behind the Alexander-de Gennes model of a planar polymer brush and summarize its major findings. We will then focus on the general impact of this seminal work by demonstrating numerous theoretical developments initiated by the Alexander-de Gennes model with specific emphasis on polyelectrolyte brushes and biological brush-like systems.

9:12AM U3.00003 Adhesion , HUGH BROWN, University of Wollongong — Adhesion is a highly practical subject in which the vast majority of published work is either chemical in nature, concerned with chemistry that is thought to occur at an adhesive junction or chemistry of adhesives, or essentially mechanical, concerned with the mechanics of testing and failure of adhesive systems. The role of polymer physics in general and de Gennes’ work in particular is to discover what happens at the scale of the polymer chain and hence form a bridge between these two approaches. A distinguishing feature of Gennes’ work in adhesion is the way he developed simple models that permitted us to see the essential physics of the situation. This is particularly true in his work in viscoelastic effects on toughness (the de Gennes trumpet) where more sophisticated mechanics had been done but the physical situation was obscure. Much of his work was concerned with the effects of connector molecules in toughening an interface in both elastomeric and glassy materials. This work has been extended by a number of authors and forms the basis of our current understanding of the area.

9:48AM U3.00004 Slippage , LILIANE LÉGER, Université Paris Sud XI — After a brief overview of the usual assumptions made to fix the boundary conditions for the flow velocity at a solid wall, we shall present the early conjecture made by Pierre Gilles de Gennes in 1979, predicting huge slip at the wall for polymer melts flowing against smooth non adsorbing surfaces. We shall then discuss how interplay between theory and experiments has allowed to produce a refined picture of the molecular mechanisms of friction at polymer interfaces, which quantitatively accounts for the three different friction regimes which have been experimentally identified when increasing the shear rate in simple shear experiments of polymer melts. The key idea (Brochard and de Gennes, 1992) focuses on the effect of a few surface anchored chains. If these chains are not rigid, they will deform under the effect of the friction forces resulting from entanglements between surface and bulk chains. When increasing the shear rate, the surface chains are thus progressively stretched, and can disentangle from bulk chains: a dynamic decoupling between surface and bulk polymer occurs. We shall discuss the available sets of experimental data (and the corresponding techniques which have been developed to either directly characterize wall slip or yield friction forces measurements). At present, the low surface density regime is fully understood, while series of data in the case of large grafting densities are available, but still lack of an adequate model. We shall finally draw lines of possible extensions of the ideas to other systems which start to be investigated as regards to friction: polyelectrolyses - grafted polyelectrolyte chains, rigid polymers, other complex fluids. We will also discuss experiments inspired by his work on confined polymers, in the last thirty years.

10:24AM U3.00005 Polymers in Confined Geometry , FRANCOISE BROCHARD-WYART, Institut Curie — Thanks to P. G. de Gennes’ famous “n = 0” theorem (relating the configuration of a polymer chain to a magnetic phase transition with an order parameter of n = 0 component), the swelling exponent ν (R = N^ν) was calculated in terms of space dimension d and fitted the qualitative Flory calculation. Using scaling laws, or the “blob” picture, it became possible to derive the configuration of a chain confined in a tube or a slit. The dynamics of confined polymers followed immediately. The new feature was the screening of the hydrodynamic interactions in confined geometry leading to Rouse-like behaviour. In a third step, de Gennes focused on the forced penetration of polymers (linear, branched, stars, neutral or charged) in narrow tubes, when they are submitted to a flow (or an electrical field for DNA). From all these calculations, the conclusion was that the threshold velocity (or field) corresponds to the penetration of the first blob. Afterwards, the friction force increases linearly with the penetrated length, whereas the confinement force remains constant. In the last few years, with his collaboration we studied the penetration of DNA in “soft” tubes. We predicted a transition from extended to globular DNA observed experimentally. We also showed that semi flexible polymer chains, like DNA, are ideal in 3d, but swollen effects are more pronounced in confined geometries. We will also discuss experiments inspired by his work on confined polymers, in the last thirty years.
and inelastic tunneling spectroscopy measurements of the electronic and dielectric properties of these high-k oxide-semiconductor systems. Using synchrotron crystal truncation rod analysis and reflection high energy electron diffraction, we place constraints on the detailed positions of the atoms at the oxide-semiconductor interface. This research has in part been motivated by a significant effort has been devoted to understand the nature of crystalline oxide-semiconductor interfaces. This research has in part been motivated by the potential applications in mind, I will also address interferometric measurements of states having superpositions of anyonic charges and discuss their non-Abelian anyonic statistics, such interferometric experiments would provide the most promising route to qubit read-out in a topological quantum computation. With these potential applications in mind, I will also address interferometric measurements of states having superpositions of anyonic charges and discuss their non-Abelian anyonic statistics, such interferometric experiments would provide the most promising route to qubit read-out in a topological quantum computation. With these potential applications in mind, I will also address interferometric measurements of states having superpositions of anyonic charges and discuss their non-Abelian anyonic statistics, such interferometric experiments would provide the most promising route to qubit read-out in a topological quantum computation. The observed quantum oscillations thus fundamentally differs from that of Aharonov-Bohm effect which has a period of one flux quantum, \( \Phi_0 \). The observed quantum oscillations in the quantum Hall corrals can be understood within the Coulomb blockade model of quantum Hall interferometers [1] as forward tunneling and backscattering, respectively, through the center island of the corral from the bulk and the edge states. In the second Landau level, we observe an extended series of oscillations with flux period of \( \Phi_0/2 \). The Aharonov-Bohm-Like oscillations are found to coexist with the \( \nu = 5/2 \) fractional quantum Hall effect. We detail the transport properties of the \( \nu = 5/2 \) fractional quantum Hall state and the mesoscopic quantum Hall corral in the second Landau level. [1] R. Rosenow and B.I. Halperin, Phys. Rev. Lett. 98, 106801 (2007).
activities taking place at IBM Zurich. It will also put them in perspective with the new rules the microelectronic industry might follow.

structures might indeed be seen as a logical conclusion for this evolution. This presentation will review the latest developments in the field, with a focus on the years ago, molecular beam epitaxy allowed band-gap engineering in compound semiconductors to build new devices and, more recently, was successfully used to explore the physics and chemistry of complex perovskites. During the last years, new developments have been made to combine oxides and semiconductors. In particular, many groups have reported the growth of oxides on silicon surfaces. The recent and renewed interest in compound semiconductor MOSFET structures might indeed be seen as a logical conclusion for this evolution. This presentation will review the latest developments in the field, with a focus on the activities taking place at IBM Zurich. It will also put them in perspective with the new rules the microelectronic industry might follow.

9:12AM U5.0003 First-principles modeling of functional oxides-semiconductor interfaces1. NA SAI, University of Texas at Austin — Search is ongoing for new classes of materials and structures based on complex oxides. One important example is the multiferroics which combine ferromagnetism or antiferromagnetism and ferroelectricity in a single phase. The coexistence, and occasionally the coupling of the two order parameters, has opened new opportunities for multifunctional applications. A promising route for practical applications is to employ thin films and multilayered structures, the properties of which can be readily manipulated at the nanoscale. Epitaxial multiferroic films are currently being developed through integration with semiconductors. Despite the progress in synthesis and experimental characterization, the roles of the interface phenomena, including strains, chemistry, etc., on the ferroelectric and magnetic properties of multiferroic thin films is not fully understood and difficult to differentiate experimentally. In this talk we illustrate the utility of theoretical methods based on density functional theory in understanding these technologically relevant structures. We describe examples of oxide-semiconductor interfaces based on YMO3 on GaN that have been synthesized recently and show how interfacial spins behave differently from those in the bulk. The interfacial effects lead to an intriguing behavior of the band offsets. We also discuss our ongoing investigation of electric field doping interfaces.

1Research in collaboration with Alex Demkov, Jaekwang Lee (University of Texas) and Craig Fennie (Argonne National Laboratory). Work at U. Texas was supported by Office of Naval Research Grant No. N000 14-06-1-0362.

9:48AM U5.0004 Thin Film Synthesis of New Complex Titanates. PAUL SALVADOR, Carnegie Mellon University — Thin film deposition methods allow for one to synthesize rationally specified compositions in targeted crystal structures. Because most of the thermodynamic and kinetic variables that control the range of materials that can be synthesized are unknown for specific compounds/processes, epitaxial stabilization and design of artificial layered crystals are driven through empirical investigations. Using examples taken primarily from the family of complex titanates, which exhibit a range of interesting physicochemical behaviors, the thermodynamic and kinetic factors that control materials design using thin film deposition are discussed. The phase competition between the pyrochlore and the (110) layered perovskite structure in the RE2Ti2O7 family (RE = rare-earth, Bi) will be explored, using pulsed laser deposition as a synthesis method. For RE = Gd, Sm, Nd, and La, the phase stability over a wide range of conditions is dictated entirely by substrate choice, indicating that the free energies of the phases are similar enough such that by controlling nucleation one controls the phase formation. In a related fashion, the growth of AE2Ti2O7 films (AE = Ba or Sr) will be discussed with respect to the formation of single-phase films or films that phase separate into AETiO3 and TiO2. The entire Ba1−xSr−xTiO3 series was grown and will be discussed with respect to growth technique (using MBE and PLD) and/or substrate choice. In this case, rock-salt substrates, which are not expected to interact strongly with any phase in the system, allow for the formation of single-phase films. Finally, several examples will be discussed with respect to the (SrO)0.5(TiO2)1.5 system, which includes the perovskite SrTiO3 and the Ruddlesden-Popper phase Sr2Ti2O5 grown using layer-by-layer molecular beam epitaxy. The solid phase epitaxial formation of the perovskite SrTiO3 from superlattices of rock-salt SrO and anatase TiO2 is discussed from both a kinetic and thermodynamic perspective by exploring the growth of a range of m and n values. Using similar arguments for stability, new layered intergrowths in the Sr2−3mTi2O5+n family are presented and their structures are discussed.

10:24AM U5.0005 Semiconductor-on-epitaxial insulator: towards ultrathin and nonclassical semiconductor devices1 ALEXANDER ZASLAVSKY, Brown University — The microelectronics industry is currently moving from bulk Si field-effect transistors (FETs) with silicon-dioxide gate insulators to high-k gate dielectric FETs and semiconductor-on-insulator (SOI) substrates, with alternative non-Si channel materials and nonplanar device layouts on the horizon. The possibility of integrating epitaxial insulator layers with well-controlled bandgaps and near-monolayer thickness control may open up new opportunities for nonclassical devices and possibly optical sources. Unlike their III-V counterparts, where epitaxial heterostructures have been available for decades, epitaxial oxide-based SOI devices have the crucial advantage of potential integrability with dominant silicon technology. This talk will discuss the examples of tunneling FETs and real-space transfer devices, as well as a proposed tunneling-based SOI intersubband laser. At this point, all of the proposed devices require epitaxial control and material quality that exceeds the state-of-the-art. Still, the unique characteristics derived from quantum mechanical tunneling make such devices an interesting playground for innovative device research, essentially replicating the III-V heterostructure device platform in the silicon-dominated microelectronics industry just as standard Si FET technology heads towards the long-predicted end of the miniaturization paradigm.

1Work in collaboration with IBM Research, LETI-Minatec (Grenoble, France), and SUNY-Stony Brook; NSF supported via ECCS-0701635 and DMR- 0302222.

Thursday, March 13, 2008 8:00 AM – 10:24 AM
Session U6 DCOMP: Computational and Theoretical Challenges in Predicting Climate Change
Morial Convention Center R04

8:00AM U6.00001 Radiative Transfer in Climate Models. VENKATACHALAM RAMASWAMY, NOAA/ GFDL Princeton University — Radiation is a key physics element in both the maintenance of the climate as well as in driving climate change. The absorption of the Sun’s radiant energy by the atmosphere- system in the ultra-violet, visible and near-infrared spectral regions, and the absorption and emission of infrared radiation by the surface and atmosphere, together govern the planetary energy balance. The importance of radiative processes enters in both the “forcing” of the climate system and in the “feedbacks” that amplify the response to perturbations of the energy balance. As examples, we will examine the natural and anthropogenic radiative forcings that have occurred over the 20th century, our understanding of the governing processes and the challenges in representing them in climate models. The quantitative description comprises the determination of the forcing at the surface and in the atmosphere due to: emissions of the long-lived greenhouse gases (e.g., carbon dioxide), ozone precursors, and pollution particulates (e.g., sulfate and black carbon); changes in land surface properties; changes in solar irradiance; and particulates arising due to episodic volcanic eruptions. The various types of forcings are governed by fundamentally different underlying mechanisms, have distinct space-time dependencies and uncertainties, and exert varying signatures in terms of the climate system responses.
8:36AM U6.00002 Climate Feedbacks and Their Simulation in Coupled Ocean Atmosphere Models, BRIAN SODEN, University of Miami — The response of Earth’s climate to an increase in greenhouse gases depends on a complex superposition of feedback processes. These processes act to either amplify or dampen the climate’s response to an initial perturbation in the Earth’s radiative energy budget. Differences in the representation of these feedback processes in current models represent a primary source of uncertainty in model projections of future climate change. Progress in reducing uncertainties in model predictions of climate change therefore requires an accurate assessment of the differences in various feedback strengths between models. In this talk I will review the key climate feedback processes and assess their range of values in current models. Attention will be focused on the feedbacks from water vapor and clouds, which represent the most important climate feedbacks in current models. My presentation will describe the prevailing view behind these feedbacks and review observational evidence used in assessing the fidelity of their representation in current models.

9:12AM U6.00003 Objective methods for detecting climate change and attribution of causes, BENJAMIN SANTER, Lawrence Livermore National Laboratory — No abstract available.

9:48AM U6.00004 Predicting climate change: Uncertainties and prospects for surmounting them, MICHAEL GHL, Ecole Normale Supérieure, Paris, France, and University of California, Los Angeles, USA — General circulation models (GCMs) are among the most detailed and sophisticated models of natural phenomena in existence. Still, the lack of robust and efficient subgrid-scale parameterizations for GCMs, along with the inherent sensitivity to initial data and the complex nonlinearities involved, present a major and persistent obstacle to narrowing the range of estimates for end-of-century warming. Estimating future changes in the distribution of climatic extrema is even more difficult. Brute-force tuning the large number of GCM parameters does not appear to help reduce the uncertainties. Andronov and Pontryagin (1937) proposed structural stability as a way to evaluate model robustness. Unfortunately, many real-world systems proved to be structurally unstable. We illustrate these concepts with a very simple model for the El Niño–Southern Oscillation (ENSO). Our model is governed by a differential delay equation with a single delay and periodic (seasonal) forcing. Like many of its more or less detailed and realistic precursors, this model exhibits a Devil’s staircase. We study the model’s structural stability, describe the mechanisms of the observed instabilities, and connect our findings to ENSO phenomenology. In the model’s phase-parameter space, regions of smooth dependence on parameters alternate with rough, fractal ones. We then apply the tools of random dynamical systems and stochastic structural stability to the circle map and a torus map. The effect of noise with compact support on these maps is fairly intuitive: it is the most robust structures in phase-parameter space that survive the smoothing introduced by the noise. The nature of the stochastic forcing matters, thus suggesting that certain types of stochastic parameterizations might be better than others in achieving GCM robustness. This talk represents joint work with M. Chekroun, E. Simonnet and I. Zaliapin.

Thursday, March 13, 2008 8:00AM - 11:00AM — Session U7 Fed: Physics Demonstrations and Strategies for Teaching and Public Outreach Morial Convention Center R05

8:00AM U7.00001 Bringing Nano to the Public through Informal Science Education, WENDY CRONE, Univ. of Wisconsin - Madison — Researchers in nanoscale science and engineering communicate all the time. We give talks, present lectures, and write papers regularly. But the general public—the consumers who will use the products of our work and the voters who indirectly set the national research agenda—do not often hear us. Informal science education—including museums, TV, public lectures, popular press, etc.—is a way to connect with broader audiences in a variety of fun and effective ways. Museums, which are visited by hundreds of millions of people each year in the U.S., are popular because they are skilled at making abstract and complex phenomena comprehensible to people from all walks of life and at making the whole experience fun. This talk will provide an introduction the “informal science education” field, discuss the art of honing your message into clear and realistic learning goals, describe methods for understanding your audience and their background, and help researchers to appreciate the limits of what can be learned in one experience. It will also review what the public currently understands about nanoscale science and engineering and the challenges that these (mis)understandings create for museums and researchers.

8:36AM U7.00002 Preparing minority undergraduate students for successful science careers, MURTY AKUNDI, Xavier University of Louisiana — Xavier University of Louisiana is well known for being number one in graduating the most minority students in physical and biological sciences. The reason for this success is built on the concept of Standards with Sympathy in the Sciences (Triple S). This is an outgrowth of over twenty years of planning and development by the Xavier science faculty to devise a program for preparing and retaining students in the sciences and engineering. Xavier has been successfully conducting for over ten years, Summer Science Academy (SSA) for middle and high school students; Science Technology, Engineering and Mathematics (STEM) Scholars and Howard Hughes Biomedical programs for in-coming freshmen. Recently, through a grant from NSF, we have developed the Experiential Problem-solving and Analytical Reasoning (EPsAR) summer bridge program for in-coming freshmen who were given conditional admission to the university (i.e., those students who scored below the acceptable range for placement into degree mathematics courses). In this program, EPsAR participants will be engaged in problem-solving and critical thinking activities for eight hours per day, five days per week, for six weeks. Additionally, an interdisciplinary approach is taken to convey the mathematical skills learned to relate to physics, chemistry, biology, and computer science. Sixty-six students have participated in the last two years in the EPsAR program. During the first year 23 of 28 students successfully bi-passed the algebra review course and were placed into a degree credit course in mathematics. In the second year, thirty-one (31) of the 38 were advanced to a higher-level mathematics course. Twenty-three (23) out of 38 went on to degree credit math course. To retain students in the sciences peer tutoring in all the science disciplines are provided. Objective methods for detecting climate change and attribution of causes, BENJAMIN SANTER, Lawrence Livermore National Laboratory — No abstract available.

9:12AM U7.00003 “Wow” is good, but “I see” is better - techniques for more effective Physics demonstrations, STEPHEN COLLINS, Academy of the Sacred Heart — The use of demonstrations to assist in Physics education at all levels is commonplace, but frequently lacks optimal effectiveness. In many cases, the choice of demonstration is not at issue, but rather the manner in which it is presented to the audience. Modern educational research reveals a number of simple ways to improve instruction of this kind, including objective setting, audience evaluation, concept building, and promoting engagement. These techniques and considerations will be reviewed, explained, and modeled through a demonstration of “Why Mr. Fork and Mr. Microwave Oven don’t get along.”

9:48AM U7.00004 Gravity - The Engine of the Universe, JOHN THACKER, California Institute of Technology — The pervasive nature of gravity ought to give us pause. Since gravity is inescapable, one could reasonably claim that it is an overarching theme in our universe. In this session we will investigate some demonstrations and strategies for teaching gravity concepts. We will use education research results on student misconceptions related to gravity to focus the activities.
Local perturbation caused by a particle driven through a 2-D colloidal suspension, CARA HAGEMAN, VIKRAM PRASAD, ERIC R. WEEKS, Emory University — When polystyrene colloids are placed at a decane-water interface they form different phases based on their area fraction. These phases are: liquid, liquid-hexatic, hexatic and crystalline. In particular, the hexatic-crystal transition is characterized by a change in the functional form of the correlation functions and the density of defects. We study this system for area fractions near the hexatic-crystal transition. Using a laser tweezer we trap and drag a particle along the interface and observe its effect on the surrounding colloids. We observe a change in the local density of defects and a decay in the perturbed motion of colloids away from the trapped particle, revealing a length scale. We measure this length scale as a function of area fraction of the colloids and the applied velocity of the trapped particle.

Micro rheology of a sticking transition, SHOBO BHATTACHARYA, PRERNA SHARMA, SHANKAR GHOSH, Tata Institute of Fundamental Research, Mumbai, India 400005 — The phenomenon of colloidal deposition in presence of shear is studied by using an optical tweezer to hold a colloidal particle in close proximity of a plate subject to a sinusoidal in-plane shaking. Through the measurement of the real and imaginary parts of the particle’s response function, the coupling between the particle and the plate is found to evolve from a viscous regime to an elastic regime through an intermediate regime of time-dependent enhancement of viscoelasticity, reminiscent of aging in glasses. The sticking transition can be described in a scenario of hindered Stokes-Einstein diffusion and the Maxwell model of viscoelasticity. Upon changing the bead-plate interaction or the strength of the drive, three regimes of response: stick, stick-slip and slip are observed. The observed behavior has analogies to jamming in granular materials and the glass transition in viscous liquids.

A New Diffusion NMR Experimental Model System for Studies of Bidisperse Colloids, ANAND YETHIRAJ, SWOMITRA PALIT, Department of Physics and Physical Oceanography, Memorial University of Newfoundland — A method to prepare monodisperse colloidal particles that are simultaneously NMR-visible and fluorescent is described. A systematic approach to obtain spectrally resolved diffusion coefficients for every component (colloid and solvent) in a monodisperse colloidal suspension is presented. We also prepared bidisperse colloidal suspensions where each colloid component has a distinct NMR spectral signature, and obtained the diffusion coefficient of both colloid species and solvent simultaneously, in concentrated colloidal suspensions with volume fractions between 20 and 50%. This colloidal model system enables the study of bidisperse colloids at different size ratios and number ratios.

Universal exponential tails in the displacement distribution observed in an attractive colloidal glass, YONGXIANG GAO, MARIA KILFOIL, McGill University — Dynamical heterogeneities exist ubiquitously in glassy materials. They manifest themselves as a non-Gaussian distribution of the constituent particle displacements, that is, the self part of the van Hove correlation function. Though the shape of the tail of the distribution looks exponential or nearly exponential, not until recently has serious attention been paid to it. We observe pure exponential behavior—neither stretched nor compressed—over a wide range of volume fractions and time scales in an attractive colloidal system on the route to attractive glass transition. We observe universal behavior as all the distributions over a wide range of \( r \) and \( \phi \) can be scaled together. The tails arise from the mobile sub-component of the constituent particles. If time permits, I will also show our studies on the structure of colloidal gels and attractive glasses in terms of a translational order parameter and an orientational order parameter, under different interaction strength, volume fraction and buoyancy matching conditions.

Point response of a 2D packing of soft colloidal spheres near the jamming transition, PETER J. YUNKER, DANIEL T. N. CHEN, ZEXIN ZHANG, ARJUN G. YODH, University of Pennsylvania — We have created a 2D jammed packing by confining a bidisperse mixture of thermo-responsive NIPA microgel spheres between two glass slides with a thickness of roughly the larger sphere diameter. The packing is subjected to a point compression created by local heating with optical tweezers. We use particle tracking microscopy to characterize the response as a function of particle volume fraction both above and below the jamming transition.

Local perturbations of dense colloidal suspensions, GIANGUIDO C. CIANCI, ERIC R. WEEKS, Department of Physics, Emory University — A rapid temperature quench can transform a liquid into a disordered solid: a glass. We model glassy materials using the mobile sub-component of the constituent particles, where the transition is induced by increasing the number density rather than decreasing temperature. This transition has drawn significant attention because it poses numerous fundamental questions. For example, close to the glass transition temperature a small decrease in temperature can cause the viscosity of the liquid to increase by 14 orders of magnitude. Meanwhile the structure remains essentially unchanged — there is no growing static length scale accompanying the transition. Fast laser scanning confocal microscopy allows us to directly observe and track thousands of colloidal particles in real time. We add a small number of superparamagnetic colloids in the sample and pull them with an external magnet. The motion of a magnetic probe locally perturbs the dense suspension and highlights its heterogeneous structure. We examine the dependence of the affected region’s size on density and applied magnetic force.

Understanding the dynamics of closely packed microgel particles, MELAKU MULUHE, HANS WYSS, GIOVANNI ROMEO, JOHAN MATTSSON, ALBERTO FERNANDEZ-NIEVES, JINWOONG KIM, DAVID WEITZ, Harvard University, WEITZ COLLABORATION — Soft particles such as microgel suspensions have important applications in industry, which exploit their unusual structural and rheological properties. Despite their relevance, the fundamental physics that controls their behavior remains poorly understood. Intriguingly, microgels act as fluid even at high density. Techniques such as rheology, microscopy, and light scattering have been used to probe the macroscopic properties of these materials — however, the underlying physical mechanisms demand further investigation. We use confocal microscopy to image the local dynamics of highly packed microgels. The gel particles are tracked over time to obtain information about the short and long range correlations of the local particle motion. We probe their response to changes in environmental factors such as temperature or pH using light scattering. The results obtained not only help us understand the origins of the observed macroscopic behavior, but also give us information on the dynamics of glassy arrest in general.
9:24AM U8.00008 Colloidal Particle Geometry and Its Effect on Optical Trapping. RACHAEL HARPER, ALEX LEVINE, Department of Chemistry & Biochemistry, University of California Los Angeles — Recent experiments by Wilking and Mason (Europhysics Letters, in press) on the laser trapping of colloids of various shapes (the letters of the alphabet) show that for identical chemistries the trapping force varies wildly with particle shape. In fact, certain shapes do not trap at all. Motivated by these experimental results, we explore the trapping of particle of variable shape using a ray-optics simulation. This numerical tool allows us to perform Monte Carlo integrations of the total trapping forces and torques for a series of objects such as a cross (the letter “x”) or a beam (the letter “I”). We find that certain shapes feature bi-stable trapping positions/orientations, and some, indeed, do not allow for trapping at all.

9:36AM U8.00009 Modeling pore formation in lipid membranes via Janus nanoparticles. ALEXANDER DEXEY, Georgia Institute of Technology, WILLIAM E. USPAL, MIT, ANNA C. BALAZS, University of Pittsburgh — Phospholipid membranes, which separate the cytoplasm from the extracellular environment in biological cells, embed a large diversity of proteins. Some proteins form pores for the free transport of small molecules and ions across the membrane. Here, we use coarse grained numerical simulations to design a synthetic membrane, where pores can be formed “on demand.” Specifically, we use dissipative particle dynamics to probe the interaction between bilayer membranes and nanoparticles. The particles are nanoscopic Janus beads that comprise both hydrophobic and hydrophilic portions. We demonstrate that when the membrane is ruptured due to an external stress, these nanoparticles diffuse to the free edge of the membrane and form stable pores, which persist after the stress is released. Pore size depends on the architecture and concentration of the nanoparticles. Once a pore is formed, a small increase in membrane tension readily reopens the pore allowing rapid transport through the membrane.

9:48AM U8.00010 Three Dimensional Rotational Motion of Colloidal Clusters. JUSTIN CARAM, Harvard University, Department of Chemistry and Chemical Biology, VINOTHAN MANOHARAN, Harvard University, Department of Physics and School of Engineering and Applied Sciences — We will present the results of a study into the three dimensional rotational and translational diffusion of colloidal clusters, especially dimers and trimers. We will have accomplished this study using both diffraction pattern and holograph analysis, as well as depolarized dynamic light scattering. We believe that trimers break into discrete rotational diffusion constants dependent on their geometries. These findings can be matched to the results for the rotational decay in the correlation function generated by DDLS. Understanding these diffusion constants is important to the understanding of protein and liquid crystal dynamics in solution. Furthermore, developing depolarized dynamic light scattering experimental strategy for non ellipsoidal systems may help to determine 3-dimensional hydrodynamic extent of such systems in solution.

10:00AM U8.00011 Anomalous Rotation of a Pair of Spherical Particles in AC Electric Fields. PUSHKAR LELE, ERIC FURST, University of Delaware — Suspensions of colloidal particles are observed to form angled bands and vortices near surfaces in AC electric fields. We map the critical frequencies and field biases at which particles phase separate into to bands and the vortices gradually set in. The results from such mapping experiments are interpreted based on measurements of anomalous rotation on a pair of colloidal particles held in blinking optical tweezers. Our observations suggest that particle pair rotation is the characteristic motion in vortices and that the polarization of double layer around the particles influences the angular velocity of the vortex evolution. Increasing the electrolyte concentration of the medium or the frequency of the electric field results in reduction of the rotation. Based on these results, the suspension behavior can be “tuned” by changing the ionic strength, field strength, field frequency and particle size.

10:12AM U8.00012 Interferometric and holographic imaging combined: correlating interface deformations with 3D tracking of interfacial particles. DAVID KAZ, VINOTHAN MANOHARAN, Harvard University — We employ the techniques of digital holography and interference phase mapping to investigate particles on interfaces. Digital holography is used to track the positions of small (micron sized) particles to within a few nanometers in three dimensions, while optical interferometry maps interfacial deformations to within a few tens of nanometers. By utilizing both techniques simultaneously, we correlate the 3D position of particles trapped on an interface with deformations of that interface at up to 1000 frames per second. Such comprehensive data will serve to answer questions regarding the capillary interactions of particles on an interface.

Thursday, March 13, 2008 8:00AM - 11:00AM — Session U9 DCMP: Fluctuations, Phase Transitions and the Polar Kerr Effect Morial Convention Center RO7

8:00AM U9.00001 Fluctuations, mean-field $T_c$ and energy gaps in cuprate superconductors. JEFFERY TALLON, Industrial Research Ltd, JAMES STOREY, Victoria University of Wellington, JOHN LORAM, Cambridge University — We have carried out an analysis of Gaussian fluctuations about $T_c$ in the specific heat of (Y,Ca)Ba$_2$Cu$_3$O$_{y-3}$ and Bi$_2$Sr$_2$CaCu$_2$O$_{y+1}$. The analysis employs a full ARPES derived dispersion, including the pseudogap. This enables us to calculate the doping dependence of the mean-field transition temperatures, $T^{mf}_c$, in the absence of fluctuations. The values lie well above $T_c$, especially for lower doping where $T^{mf}_c$ is trending towards 180K. As a result, while the observed $T_c$, follows the well-known parabolic doping dependence, the values of $T^{mf}_c$ decrease monotonically with doping along with the superconducting gap parameter, $\Delta_0$, such that $2\Delta_0/k_BT_c \sim 0.3$. Using this result, we offer explanations for a number of anomalous observations. The line $T^{mf}_c(p)$ should not however be confused with the $T^*(p)$ line which is associated with the pseudogap and falls abruptly to zero at critical doping ($p_{crit}=0.19$ holes/Cu).

8:12AM U9.00002 Universal values for the static and dynamic critical exponents in thin-film and bulk crystalline YBCO. C.J. LOBB, SU LI, HUA XU, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, M.C. SULLIVAN, Department of Physics, Ithaca College, Ithaca, NY. K. SEGAWA, YOICHI ANDO, ISIR, Osaka University, Ibaraki, Osaka, Japan, S.M. ANLAGE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — Many researchers have used scaling of current vs. voltage curves to study the normal-superconducting phase transition of the high-temperature superconductors, searching for the static and dynamic critical exponents; however, there is little consensus among experimentalists as to the values of the exponents. We have studied this phase transition in optimally-doped YBa$_2$Cu$_3$O$_{y-3}$ thin films and bulk crystals. We consistently find $\nu = 1.5 \pm 0.2$ for the dynamic critical exponent in films (when finite-size effects are taken into consideration) and in crystals (where there are no finite size effects). We also find for the static critical exponent $\nu = 0.63 \pm 0.1$ for crystals and $\nu = 0.63 \pm 0.1$ for films. The failure to account for finite-thickness effects in thin films may account for the wide ranges of values for $\nu$ and $\Delta$ previously reported in the literature.}

1Supported by NSF grants DMR-0302596 and DMR-0706557.
8:24AM U9.00003 Dynamic critical behavior of YBCO thin films/crystals. HUA XU, SU LI, CHRISTOPHER LOBB, STEVEN ANLAGE, Center for Nanophysics and Advanced Materials, University of Maryland, College Park — The zero-field phase transition of high-Tc superconductors has been studied by a number of techniques. However transport properties (such as the conductivity) which probe the dynamics near Tc are less explored, and a wide range of critical exponents have been reported experimentally. We studied fluctuation effects of YBa2Cu3O7-δ thin films around Tc by doing frequency-dependent microwave conductivity and DC nonlinearity measurements. The length scales involved in the measurements and their influence on the fluctuation conductivity have been examined systematically, and this helps to clarify the historical discrepancy between experimental results and scaling predictions. Our results give a dynamical scaling exponent $z = 1.55 \pm 0.15$, which indicates the superconducting to normal phase transition of high-Tc materials likely belongs to the model E-dynamics.

This work was supported by NSF grant number DMR-0302596.

8:36AM U9.00004 Two-Dimensional Superconducting Fluctuations in Stripe-Ordered La$_2$-xBa$_x$CuO$_4$. QIANG LI, Brookhaven National Laboratory, MARKUS HUCKER, GENDA GU, ALEXEI TSVELIK, JOHN TRANQUADA — Recent spectroscopic observations of a d-wave-like gap in stripe-ordered La$_2$-xBa$_x$CuO$_4$ with x=1/8 have led us to critically analyze the anisotropic transport and magnetization properties of this material. The data suggest that concomitant with the spin ordering is an electronic decoupling of the CuO$_2$ planes. We observe a transition (or crossover) to a state of two-dimensional (2D) fluctuating superconductivity. Thus, it appears that the stripe order in La$_2$-xBa$_x$CuO$_4$ frustrates three-dimensional superconducting phase order, but is fully compatible with 2D superconductivity and an enhanced $T_c$ — [Ref. Q. Li et al., PRL 99, 067001 (2007)]

8:48AM U9.00005 Disorder-induced quantum critical point in an anisotropic gap superconductor. VICTOR GALITSKI, Physics Department and Joint Quantum Institute, University of Maryland — We consider an inhomogeneous anisotropic gap superconductor in the vicinity of the quantum critical point, where the transition temperature is suppressed to zero by disorder. Starting with the BCS Hamiltonian, we derive the Ginsburg-Landau action for the superconducting order parameter. It is shown that the critical theory corresponds to the marginal case in two dimensions and is formally equivalent to the theory of an antiferromagnetic quantum critical point, which is a quantum critical theory with the dynamic critical exponent, $z=2$. This allows us to use a parquet method to calculate the non-perturbative effect of quantum superconducting fluctuations on thermodynamic properties. We also discuss mesoscopic disorder fluctuations, which lead to the spatial variations of the local pairing temperature and the formation of superconducting islands above the mean-field transition. This disorder-induced Griffiths phase is described by a network of superconducting islands and metallic regions with a strongly suppressed density of states due to superconducting fluctuations. We argue that the phenomena associated with mesoscopic disorder fluctuations may also be relevant to high-temperature superconductors, in particular, to recent STM experiments, where gap inhomogeneities have been explicitly observed.

9:00AM U9.00006 Fermi arcs in phase fluctuating d-wave superconductors. EHUD ALTMAN, Weizmann Institute, EREZ BERG, Stanford University — One of the most puzzling aspects of the high-Tc superconductors is the appearance of Fermi arcs in the normal state of the underdoped cuprate materials. These are loci of low energy excitations covering part of the Fermi surface, that suddenly appear above $T_c$ instead of the nodal quasiparticles. Based on a semiclassical theory, we argue that partial Fermi surfaces arise naturally in a d-wave superconductor that is destroyed by thermal phase fluctuations. Specifically, we show that the electron spectral function develops a square root singularity at low frequencies for wave-vectors positioned on the bare Fermi surface. We predict a temperature dependence of the arc length that can partially account for results of recent angle resolved photo emission (ARPES) experiments.

9:12AM U9.00007 Vortex dynamics and Nernst effect in fluctuating superconductors. DANIEL PODOLSKY, University of Toronto, SRINIVAS RAGHU, Stanford University, ASHVIN VISHWANATH, University of California at Berkeley, DAVID HUSE, Princeton University — We present a new method to study the Nernst effect and diamagnetism of an extreme type II superconductor dominated by phase fluctuations. We work directly with vortex variables and our method allows us to tune vortex parameters (eg. core energy and number of vortex species). We find that diamagnetic response and transverse thermoelectric conductivity ($\sigma_{xy}$) persist well above the Kosterlitz-Thouless transition temperature, and become more pronounced as the vortex core energy is increased. However, they weaken as the number of internal vortex states are increased.

9:24AM U9.00008 Nernst effect in the phase-fluctuating superconductor InO. PANAYOTIS SPATHIS, HERVE AUBIN, ALEXANDRE POURRET, CIGDEM CAPAN, KAMRAN BEHNIA, ESPCI — We present a study of the Nernst effect in the amorphous superconductor InO. The low carrier density in this system implies a weak superfluid stiffness and consequently, strong phase fluctuations of the superconducting order parameter are expected. Measurements as function of temperature show that the Nernst signal evolves continuously through the superconducting transition as previously observed in underdoped cuprates. This contrasts with the abrupt jump expected at a BCS transition, as observed previously in Nb$_{0.15}$Sn as. In the last system, the Nernst signal due to vortices below $T_c$ and by Gaussian fluctuations above are clearly distinct [1]. The behavior of the ghost critical field in InO points to a correlation length which does not diverge at the Cooper-pair forming temperature $T_c$, a temperature below which the amplitude fluctuations freeze, but phase fluctuations survive. [1] Pourret et al, Nature Physics 2, 683 (2006)

9:36AM U9.00009 Bosonic Field Driven Superconductor-Insulator Transitions in Amorphous Nano-honeycomb Films. M.D. STEWART, JR., AIJUN YIN, J.M. XU, JAMES M. VALLES, JR., Brown University — We have observed multiple magnetic field driven superconductor-insulator transitions (SIT) in amorphous Bi films perforated with a nano-honeycomb (NHC) array of holes. The magneto-resistance across the SITs is periodic, with a period $H = H_M = h/2eS$, where $S$ is the area of a unit cell of holes. These transitions are, therefore, boson dominated. In constant field the temperature dependence of the resistance can be parameterized by $R(T) = R_0(T) \exp(T_c(T)/T)$ on both sides of the transition so that the evolution between the superconducting and insulating states is controlled by the vanishing of $T_c(T)$. We compare these data to the thickness driven transition in NHC films and the field driven transitions in unpatterned Bi films, other materials, and Josephson junction arrays. Our results suggest a structural source for similar behavior found in some materials and that despite the clear bosonic nature of the SITs, quasiparticle degrees of freedom likely also play an important part in the evolution of the SIT.

This work supported by the NSF through DMR-0606597 and DMR-0203608 and by the AFRL and ONR.

9:48AM U9.00010 Excess Voltage Noises in the Superconducting Transition in Thin Films. HENGSONG ZHANG, FULIN ZUO, University of Miami — We report voltage noise studies in the superconducting transition of thin Sn films. Voltage noises are measured as a function of temperature and applied current. The noise spectral power $S^{1/2}$ is peaked during the superconducting transition, with the peak temperature shifted downward from that of dR/dT. Comparison with the dc noise measurement shows the $S^{1/2}$ is much larger with ac current than dc. I-V characteristics and voltage noises are measured simultaneously to correlate the voltage noise with the vortex motion. The noise depends on the voltage with a characteristic $\sqrt{V}$ dependence for small V, suggesting shot noise nature for the excess noises.
10:12AM U9.00012 Kerr Effect in Superconductor. SANG BOO NAM — A magnetic field \( H \) is to make the time reversal symmetry break. By using the formulation [1], neglecting \( H \) dependence of \( \Delta(T) \) and for the pair cyclotron frequency \( \Omega = (2e/2m)h/c \) less than the photon frequency \( 2\pi c/\lambda \), the Kerr angle is obtained as \( \theta_K(T) = \theta_K(0)[(\Delta(T)/\Delta(0))\tanh(\Delta(T)/2k_BT)] \), where \( \theta_K(0) = \Delta^3 / \Omega^2 / (8\pi^3 N \lambda^2) \), \( \lambda = (3\delta/4, L)\delta_{BCS} \) in the (non-local, local) limit, with mean free path length \( L \) and BCS coherence length \( \xi_{BCS} \) for the pair in the normal state. We consider the effects of the Berry phase on the formation of the flux patterns in mesoscopic type-I SC using the phenomenological Ginzburg-Landau theory. We carry out simulations on three-dimensional samples of different geometries. We show that in the samples with sharp boundaries the amplitude of the \( d_{xy} \) admixture is quite small compared to the ordered DDW component.


10:24AM U9.00013 Possible Weak Ferromagnetism in Time Reversal Violating State of Underdoped Cuprates. VIVEK AJI, CHANDRA VARMA, University of California, Riverside — Recent polar Kerr effect measurements on underdoped \( \text{YBCO} \) have provided evidence for time reversal symmetry breaking near the pseudogap temperature. These results are consistent with the existence of a ferromagnetic moment of order \( 10^{-11} \) Bohr magneton along the \( c \)-axis. We discuss the conditions for the possible occurrence of ferromagnetism with moments perpendicular to the Copper-Oxideplanes, accompanying the loop current orbital magnetic order, in the underdoped phase of Cuprates.

10:36AM U9.00014 Electromagnetic response of a chiral \( p \)-wave superconductor. RAUL ROY, JOHN BERLINSKY, CATHERINE KALLIN, McMaster University — We study the response of a time-reversal symmetry breaking \( p_x + ip_y \) superconductor to an external electromagnetic wave and calculate the ac Hall conductivity, paying particular attention to the Kerr angle. For the topological Chern Simons term in the effective action and contributions from collective modes. We also consider the effects of a long range interaction such as the Coulomb interaction on the collective modes and the Hall conductivity. These results will also be discussed in the context of recent Kerr rotation experiments on Strontium Ruthenate by Xia et al. [1].


10:48AM U9.00015 Absence of magnetic field \( (B \leq 33 \text{ T}) \) induced effects in the mid-infrared properties of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) films with \( 0 \leq x \leq 0.16 \). S.V. DORDEVIC, L.W. KOHLMAN, The University of Akron, A. GOZAR, G. LOGVENOV, I. BOZOVIC, Brookhaven National Lab, L.C. TUNG, Y.-J. WANG, National High Magnetic Field Lab — We have performed magneto-transmission measurements on a series of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) films with magnetic fields up to 18 Tesla. Studied samples include doping levels \( x = 0 \), \( 0.1 \), \( 0.3 \), \( 0.45 \), \( 0.6 \), \( 0.8 \), \( 0.10 \). In addition, an optimally doped film \((x=0.16)\) was studied in magnetic fields as high as 33 Tesla, both below and above its superconducting critical temperature \( T_c = 41 \text{ K} \). In neither of the studied samples we could detect any field-induced changes of transmission in the mid-infrared energy range (between about 1000 and 3500 cm\(^{-1}\)). We discuss how these observations can enhance our current understanding of energy range excitations in the cuprates, and their relation to high temperature superconductivity.

Thursday, March 13, 2008 8:00AM - 10:48AM - Session U10 DCMP: Superconductivity: Magnetic Field Effects

8:00AM U10.00001 Peak Effect in \( \text{Co}_x\text{NbSe}_2 \) Single Crystals. MARIA IAVARONE, Argonne National Laboratory, R. DI CAPUA, Universita’ degli Studi del Molise, Italy, G. KARAPETROV, Argonne National Laboratory, A. KOSHELEV, D. ROSENMANN, H. CLAUIS, W.K. KWOK, Argonne National Laboratory — We report a pronounced peak effect in the magnetization of \( \text{Co}_x\text{NbSe}_2 \) single crystals having critical temperatures ranging between 7.1 K and 5.0 K. Magnetization studies reveal that the magnetic irreversibility below the peak effect regime is higher in samples with lower concentration of Co while exhibits a nearly reversible magnetization over a wide range of magnetic field for samples with higher concentration of Co. However, in the peak effect regime the situation is different. The irreversibility is a non-monotonic function of the Co content, and therefore of the critical temperature of the sample. This behavior cannot be explained as a crossover between collective to single pinning regimes as suggested for \( \text{NbSe}_2 \), since this should be a monotonic function of number of pinning centers. Furthermore, we investigated the peak effect regime with low temperature STM at 4.2 K and 1.8 K. [1] This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne, a U.S. Department of Energy Office of Science Laboratory, is operated under Contract No. DE-AC02-06CH11357

8:12AM U10.00002 Effect of the sample geometry on the intermediate state in mesoscopic 3D Type-I superconductors. GOLIJBON JERDiyorov, Departamento Fisica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium, ALEXANDER HERNANDEZ, Centro Atómico Bariloche, 8400 San Carlos de Bariloche, Rio Negro, Argentina, FRANCOIS PEETERS, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — The intermediate state (IS) of type-I superconductors (SC) has recently became a topic of increasing interest. [1,2]. Direct imaging of type-I SC reveals two distinct topologies of the intermediate state: flux tubes are formed upon magnetic field penetration and laminar patterns appear upon flux exit [2]. However, spheres and cones show no hysteresis with flux tubes dominating the IS [1]. In this work we investigate the effect of the sample topology on the formation of the flux patterns in mesoscopic type-I SC using the phenomenological Ginzburg-Landau theory. We carry out simulations on three-dimensional samples of different geometries. We show that in the samples with sharp boundaries (cubes and disks) laminar structures are mostly located along the boundary, whereas radial distribution of the flux patterns is obtained for cones and spheres. The effect of the edge defects on the observed structures will also be studied. [1] R.Prozorov, Phys. Rev. Lett. 98, 257001 (2007). [2] M. Menghini et al., Phys. Rev. B 75, 014529 (2007).
8:24AM U10.00003 Pauli Paramagnetic Effects on the Vortices in Superconducting TmNi$_2$B$_2$C, L. DEBEER-SCHMITT, M.R. ESKILDSEN, University of Notre Dame, M. ICHIOKA, K. MACHIDA, Okayama University, Japan, N. JENKINS, University of Geneva, Switzerland, C.D. DEVHURST, Institut Laue-Langevin, France, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory and Iowa State University — The magnetic field distribution around the superconducting vortices in TmNi$_2$B$_2$C in the paramagnetic phase above $T_N$ was studied experimentally as well as theoretically. Using small-angle neutron scattering we imaged the vortex lattice (VL). Using the magnitude of the VL scattering vector, we obtain a direct measure of the magnetic induction, $B$, which is found to exceed $\mu_0 H$ at all fields up to $H_{c2}$. Measurements of the VL reflectivity yielded a form factor which remains essentially constant up to $\sim 0.6 H_{c2}$, above which it decreases rapidly but remains measurable up to the upper critical field. This field dependence of the form factor is in striking contrast to the usual exponential suppression. The measured form factor is well fitted by model based on the Eilenberger equations, extended to include paramagnetic effects due to the exchange interaction with the localized 4$f$ Tm moments. The model shows how the induced paramagnetic moments around the vortex cores act to maintain the field contrast probed by the form factor. The results will be compared to our recent measurements of the VL form factor in CeCoIn$_5$, which also indicate strong paramagnetic effects.

8:36AM U10.00004 Pauli-Limited Superconductors with Magnetic Fluctuations, ROBERT BEAIRD, Louisiana State University, ANTON VORONTSOV, University of Wisconsin-Madison, ILYA VEKHTER, Louisiana State University — We examine the full wave vector $q$ dependence of the expansion coefficients and examine the onset of both the uniform and spatially modulated superconducting phases along critical magnetic field $B_c(T)$. In the absence of fluctuations, both superconducting transitions are second order in 2D and meet at a tricritical point $B_c(T^*)$. We find that including magnetic fluctuations introduces first order transitions into the superconducting phase. We find the tricritical points where these transitions meet and determine $B_c(T)$ and $q(T)$ as functions of the coupling between superconducting order and the fluctuating magnetization.

8:48AM U10.00005 Evidence for Field-Induced Quantum Criticality in an Overdoped Cuprate, TAKASADA SHIBAUCHI, Dep. of Physics, Kyoto University, LIA KRUSIN-ELBAUM, IBM T. J. Watson Research Center, MASASHI HASEGAWA, Department of Materials Science and Engineering, Nagoya University, YUICHI KASAHARA, RYUJI OKAZAKI, Dep. of Physics, Kyoto University, YUJI MATSUDA, Dep. of Physics, Kyushu University, and ISSP, University of Tokyo — In current views, the putative quantum critical point in high-$T_c$ superconductors is understood to be driven by charge doping. Here we uncover an unexpected transition from a non-Fermi- to a Fermi-liquid state driven by magnetic field in a highly overdoped Tl$_2$Ba$_2$CuO$_{6+x}$ with $T_c \geq 15$ K. From the $c$-axis resistivity measured up to 45 T, we show that the Fermi-liquid $\rho_c = \rho_c(0) + A T^2$ features, accompanied by a (quantum) field-linear magnetoresistance, appear above a temperature-dependent field $H_{FL}(T)$, which decreases linearly with decreasing temperature and points to a quantum critical point near the upper critical field $H_{c2}(0)$. The observed field-induced quantum criticality with a power-law diverging $\rho_c(H)$ bears a striking resemblance to that of heavy-fermion superconductor CeCoIn$_5$, suggesting a common underlying physics in these strongly correlated electron systems.

9:00AM U10.00006 Superconducting Vortices in CeCoIn$_5$: Beyond the Abrikosov-Ginzburg-Landau Paradigm, A. D. BIANCHI, Dpt. de physique, U. de Montréal, Montréal, QC, Canada, M. KENZELMANN, J. MESOT, M. ZOLLIKER, J. KOHLBRECHER, LNS ETHZ & PSI, PSI, Switzerland, L. DEBEER-SCHMITT, M. R. ESKILDSEN, Dept. of Physics, U. of Notre Dame, Notre Dame, IL, USA, J. S. WHITE, E. M. FORGAN, School of Phys. and Astro., U. of Birmingham, Birmingham, UK, Z. FISK, Dep. Phys. & Astro., UC Irvine, Irvine, CA, USA, R. MOVSHOVICH, E. D. BAUER, J. L. SARRAO, MPA-10, LANL, Los Alamos, NM, USA, C. PETROVIC, Cond. Matt. Phys., BNL, Upton, NY 11973, USA — We report on the magnetic field ($H$) dependence of the form factor $|F|^2$ of the vortex lattice (VL) in CeCoIn$_5$ obtained by small angle neutron scattering for $H$ applied along the crystallographic $c$-axis. Superconductivity (SC) in CeCoIn$_5$ has several unconventional aspects to it: The $d$-wave SC is in competition with antiferromagnetic order, as suggested by the presence of an magnetic QCP located at the upper critical field $H_{c2}(0)$. The observed field-induced quantum criticality with a power-law diverging $|F|^2$ in CeCoIn$_5$ bears a striking resemblance to that of heavy-fermion superconductor CeCoIn$_5$, suggesting a common underlying physics in these strongly correlated electron systems.

9:12AM U10.00007 Reversal of specific heat oscillations with planar magnetic field in 2D d-wave superconductors: Doppler shift beyond the nodal approximation., G.R. BOYD, P.J. HIRSCHFELD, University of Florida, ILYA VEKHTER, Louisiana State University — Experiments on several novel superconducting compounds found oscillations of the specific heat when an applied magnetic field is rotated with respect to the crystal axes. The results are commonly interpreted as arising from the nodes of an unconventional order parameter, but the identifications of nodal directions are sometimes controversial. While the semiclassical method predicted the minima of $c^2$ near $\pm \pi/2$ in the $(T, c^2)$ phase diagram of a paramagnetically-limited superconductor in the presence of fluctuating magnetic moments. We derive the Landau- Landau free energy functional for the superconducting order from microscopics and include classical fluctuations of the magnetization. We consider the full wave vector $q$ dependence of the expansion coefficients and examine the onset of both the uniform and spatially modulated superconducting phases along critical magnetic field $B_c(T)$. In the absence of fluctuations, both superconducting transitions are second order in 2D and meet at a tricritical point $B_c(T^*)$. We find that including magnetic fluctuations introduces first order transitions into the superconducting phase. We find the tricritical points where these transitions meet and determine $B_c(T)$ and $q(T)$ as functions of the coupling between superconducting order and the fluctuating magnetization.

9:24AM U10.00008 Effect of Charge Carrier Density on the Vortex Regimes in Y$_{1-x}$Pr$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ Single Crystals, P. GYAWALI, V. SANDU, C.C. ALMASAN, Kent State University, B.J. TAYLOR, M.B. MAPLE, University of California at Davis — We report the evolution of the vortex matter state in the temperature and field range where the second magnetization peak SMP is present by studying the magnetization and magnetic relaxation of a series of Y$_{1-x}$Pr$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ ($x = 0.13$, $T_c = 82$ K; $x = 0.34$, $T_c = 50$ K; $x = 0.47$, $T_c = 34$ K) single crystals. Our study has shown that the main ingredient that controls the evolution of the vortex matter through the different regimes is the charge carrier density. The SMP is first enhanced and then suppressed as Pr concentration increases. The reason for this behavior is the softening of the elastic moduli, which makes the vortex lattice less stable to defect invasion. Within the collective creep theory, we determined the apparent activation energy. Its evolution with current density has shown that the vortex system is predominantly elastically pinned below the SMP, while above there is a smooth crossover to a vortex regime most likely dominated by the proliferation of dislocations.
9:36AM U10.00009 Skyrmmion Flux Lattices and their μSR signature1, QI LI, JOHN TONER, DIETRICH BELITZ, University of Oregon — Recently, topological excitations known as skyrmions were predicted to exist in p-wave superconductors [1]. The elastic theory of an induced skyrmion lattice was developed in [2], and its melting curve was found to be qualitatively different from that for vortex lattices. Here we show that the muon spin resonance (μSR) signatures of the two types of lattices are also very different. μSR has been applied extensively to study the magnetic properties of vortex flux lattices [3]. The observable in this technique is the μSR line shape \( n(B) \), which is the probability density that a muon experiences a local magnetic induction \( B \). In a vortex lattice, for small \( B \), \( n(B) \propto \ln(1/B)/B \). By contrast, for a skyrmion lattice we predict \( n(B) \propto B^1 - 3/2 \). This difference provides another way to easily distinguish between vortex and skyrmion flux lattices, and can thus help to identify p-wave superconductors. [1] A. Knigavko, B. Rosenstein, and Y.F. Chen, Phys. Rev. B 60, 550 (1999). [2] QI Li, John Toner, and D. Belitz, Phys.Rev. Lett. 98, 187002 (2007). [3] J. E. Sonier, J.H. Brewer, and R. F. Kiefl, Rev. Mod. Phys. 72, 769 (2000).

1This work was supported by the NSF under grant No. DMR-05-29966.

9:48AM U10.00010 Non-linear magnetization effects within the Kosterlitz-Thouless theory, LARA BENFATTO, Centro Fermi and University of Rome “La Sapienza”, CLAUDIO CASTELLANI, University of Rome “La Sapienza”, THIERRY GIAMARCHI, University of Geneva — Recent experiments in cuprate superconductors have attracted the attention on the role of vortex fluctuations. Measurements of the field-induced magnetization showed that the correlation length diverge exponentially, as predicted within the Kosterlitz-Thouless (KT) theory. However, it is somehow puzzling the persistence of non-linear magnetization effects at low field. Here we address this issue by means of a new theoretical approach to the KT transition at finite magnetic field, based on the sine-Gordon model. This approach is particularly useful in two respects. First, it leads to a straightforward definition of the field-induced magnetization as a function of the external magnetic field \( B \) instead of the magnetic induction \( B \), which is crucial to get a consistent description of the Meissner phase. Second, it allows us to identify the cross-over field \( H_{cr} \) from non-linear magnetization both below and above the transition. Above \( T_{KT} \), \( H_{cr} \) turns out to scale as the inverse correlation length, so that it decreases as the transition is approached. As a consequence, the fact that the only non-linear regime is accessible experimentally should be interpreted as a typical signature of the fast divergence of the correlation length within the KT theory. L.Benfatto, C.Castellani and T.Giamarchi, Phys. Rev. Lett. 99, 207002 (2007).

10:00AM U10.00011 Theory of diamagnetic response in layered superconductor above “Tc”, PEIJEN LIN, Electrophysics department, National Chiao Tung University, DINGPING LI, Beijing University, BARUCH ROSENSTEIN, Electrophysics department, National Chiao Tung University — Recent work by Wang et al. (Phys. Rev. Lett. 95, 247002) on field induced diamagnetic properties above Tc attracted a lot of attention from both theoretical and experimental physicist. In this talk, we will show that this phenomenon can be understood using conventional Ginsburg Landau theory for anisotropic materials. Above Tc, where the thermal fluctuations are strong, the effective description based on GL becomes non trivial due to the important contribution of higher landau levels. In previous works, some progress was achieved when certain additional assumptions (such as Lowest Landau Level approximation) were made. However, the validity of these assumptions is under debate. In our study of this system, we include the contribution of higher landau levels with nonperturbative method.Comparison will be made with Varlamov-Larkin results.

10:12AM U10.00012 Theory of quantum magneto-oscillations in underdoped cuprate superconductors1, SASHA ALEXANDROV, Loughborough University — Magneto-oscillations in kinetic and magnetic response functions of a few underdoped cuprates are perhaps one of the most striking observations since many probes of underdoped cuprates clearly point to a non Fermi-liquid normal state. Their observation in the vortex state well below the upper critical field raises a doubt concerning their normal state origin. Here I propose an explanation of the magneto-oscillations as emerging from the quantum interference of the vortex lattice and checkerboard modulations of the electron density of states revealed by STM with atomic resolution in some cuprate superconductors. The checkerboard effectively pins the vortex lattice, when the period of the checkerboard is commensurate with the period of the vortex lattice. This condition yields a periodicity of the response functions, rather than periodicity of conventional normal state oscillations periodic versus inverse magnetic field \( B \). Our solution of the Gross-Pitaevskii-type equation for composed charged bosons accounts for the \( d \)-wave symmetry of the order-parameter and its checkerboard modulations, and describes well changes in resonant frequency of the tunnel-diode oscillator circuit with \( \text{YBa}_2\text{Cu}_3\text{O}_6 \) and the oscillatory part of the Hall resistance in the mixed state of \( \text{YBa}_2\text{Cu}_3\text{O}_6 \).

1This work is supported by EPSRC (UK) (grant No. EP/D035589).

10:24AM U10.00013 Enhanced tunneling in a magnetic field, BORIS IVLEV — As known, a probability of quantum tunneling through a static potential barrier \( U(x) \) can be substantially reduced by a static magnetic field \( H_z \). This happens due to increase of the effective barrier height caused by Landau’s gauge potential in a magnetic field (the same potential results in Landau levels). There is an exponentially small current in the direction of tunneling, \( x \). An underbarrier current in the direction perpendicular to tunneling, \( y \), is not small. If the potential barrier \( U(x, y) \) depends also on the coordinate \( y \), a new unexpected scenario can occur. Now the partial de Broglie waves, generated under the barrier, are not collected to the current in the \( y \) direction only but can be reflected by the potential \( U(x, y) \). An interference of those underbarrier waves after reflections can result in a peak of the particle density at a classically allowed region close to the conventional exit point from under the barrier. At the critical magnetic field, \( H_z = H_{cr} \), the peak amplitude is not exponentially small (Euclidean resonance). The same phenomenon can occur in tunneling through nonstationary barriers and is expected for photon tunneling when a refractive index is slightly inhomogeneous in the tunnel region.

10:36AM U10.00014 Current induced properties in bulk YBCO above the transition temperature, GEORGE ZIMMERMAN, Boston University, Emeritus — Simultaneous measurement of the electrical resistivity at high current densities and magnetic susceptibility of YBCO superconducting material reveals interesting behavior of the samples above the transition temperature. In addition to anomalies which appear at temperatures between 85K and 140K, the susceptibility seems to be affected by the electrical current up 200K. The electrical current, of density between 8 and 400 A/cm², seems to induce the behavior, with a lowered resistivity, which suggests a first order phase transition, possibly meta-stable, and persists despite the repeated cycling between 77K and 300K. The samples of bulk polycrystalline cylindrical rods 1.22 mm diameter and between 6cm and 20 cm long have a density of 5.4 gm/cm³ and were prepared sintering and annealing from a YBCO powder. Most were 10 to 15 years old. At 77K most samples exhibit relaxation times of several minutes in their magnetic and resistive behavior. The details of the measurements as a function of temperature, current density, and low magnetic field, will be described along with possible implications as to the nature of the pseudo-gap and other competing theories.

Thursday, March 13, 2008 8:00AM - 11:00AM –
Session U11 DMP: Focus Session: MgB2-like: Enhancement of Superconducting Properties
Morial Convention Center Room 909
8:00AM U11.00001 Introduction of Carrier Scattering in MgB$_2$, and its Effect on both Normal and Superconducting Properties, especially Hc$_2$. N. NEWMAN, Y. SHEN, R. SINGH, J. ROWELL, ASU, D. LARBALESTIER, F. HUNTE, FSU — The low Hc$_2$ values seen in pure and well ordered MgB$_2$ can be raised dramatically, to 35 T or more, by introducing carrier scattering by native and impurity defects. We describe three means to do this. First, He ion irradiation is used to tune Tc from 39K to less than 10K, while at Tc near 33K, Hc$_2$ reached a maximum value. Similar behavior has been reported for neutron damage and carbon doping. Second, we introduced oxygen in the films, either in-situ or ex-situ, and again, high Hc$_2$ values were seen and in these films, very high Jc values as well. Finally, a novel route has been investigated. We deposited MgB$_2$ films on room temperature substrates, then annealed at temperature just sufficient to produce crystallinity, giving Tcs in the range of 10 to 30K. Such films exhibit large dHc$_2$/dT values near Tc, sometimes larger than 2 T/K. This work is of practical importance and gives an improved understanding of how intraband and interband carrier scattering in the “2-gap” superconductor MgB$_2$ determine its Hc$_2$, resistivity and Tc.

8:12AM U11.00002 Upper critical field enhancements of TMB HPCVD magnesium diboride, F. HUNTE, J. JAROSZYNSKI, A. GUREVICH, D.C. LARBALESTIER, Applied Superconductivity Center, NHMFL, Florida State University, Y. ZHU, P.M. VOYLES, University of Wisconsin, Madison, R.H. WILKE, X.X. XI, The Pennsylvania State University — The H$_c2$ of four well textured carbon-doped-MgB$_2$ films grown by HPCVD from tri-methyl boron (TMB) at flow rates from 2.5 to 10 sccm was measured in fields up to 45T. H$_c2$ derived from low-current, four-point magnetoresistance clearly increases with increasing TMB flow rate. TMB appears to be a more uniform dopant than the (C$_x$H$_{2-x}$)$_2$Mg used earlier. These earlier films exhibited H$_c2$($0$) up to 70 T but also were imperfectly connected ($\rho$(50K) $\approx$ 200 – 800 $\mu\Omega$cm) due to excess amorphous C-rich phases observed between the MgB$_2$ grains. In strong contrast, $\rho$(50K) was only 10 – 20 $\mu\Omega$cm for the TMB films. When first measured, the linearly extrapolated H$_c2$($0$) reached $\sim$40 T for the film with the highest TMB flow rate, but after about 3 months of aging, this value rose to $\sim$50 T. The angular dependence of H$_c2$ for this sample was measured up to 45 T yielding H$_c2$(4.2 K) = 45.8 T and showing the good Ginzburg-Landau scaling with an H$_c2$ anisotropy of 2.88 at 4.2 K. These results are discussed in terms of the theory of dirty two-gap superconductors as a part of an in-depth study of the effect of ternary doping of magnesium diboride.

8:24AM U11.00003 Kinetic roughening of magnetic flux penetration in MgB$_2$ thin films, ANDREA LUCARELLI, GUNTER LUEPKE, College of William and Mary, BRIAN MOECKLY, Superconductor Technologies, Inc., YUE ZHAO, SHI DOU, University of Wisconsin, Madison, Wisconsin, R. ANSCHITZ, and L. KOWALSKI, University of Wisconsin, Madison — MgB$_2$ thin films exhibit pronounced instabilities such as finger-like structures, flux jumps or dendritic patterns, which endanger electronic devices at high field. This effect can be correlated to the defects that were induced by irradiation. In fact TEM images show the presence of amorphous regions whose sizes are compatible with the coherence length and such as to act as pinning centers through two different mechanisms. The influence that longitudinal and transverse resistivity of seven different samples with variable disorders characterized by the residual resistance ratio ($\rho$(0)/$\rho$(T)) measured in fields up to 45 T at different temperatures.

8:36AM U11.00004 Evidence of new pinning centers in irradiated MgB$_2$, C. TARANTINI, A. MARTINELLI, P. MANPRINNETTI, A. PALENCIO, I. PALLECHI, M. PUTTI, C. FERDEGHI, CNR-INFN-LAMIA, University of Genova, Via Dodecaneso 33, 16146 Genova, Italy, M.R. CIMBERLE, CNR-IMEM, Via Dodecaneso 33, 16146 Genova, Italy — It has been shown that C or SiC additions can strongly enhance upper critical field of MgB$_2$, leading to an in-field increase of critical current, but without introducing pinning centers other than grain boundaries. On the contrary neutron irradiation introduces new pinning centers, as highlighted by a significant shift of the maximum of pinning force and by a strong improvement of Jc at high field. This effect can be correlated to the defects that were induced by irradiation. In fact TEM images show the presence of nanometric amorphous regions whose sizes are compatible with the coherence length and such as to act as pinning centers through two different mechanisms. The influence that neutron irradiation induces on MgB$_2$ is also confirmed by magnetization decay tests that, differently by doped samples, show an important enhancement of pinning energies at high field. These measurements highlight as the increase of pinning energy with irradiation flux is strongly correlated with Jc improvement.

8:48AM U11.00005 Flux Pinning and Connectivity in MgB$_2$, M.D. SUMPTION, M. SUSNER, M. BHATIA, E.W. COLLINGS, Materials Science Department, Ohio State University — The transport and pinning properties of in-situ MgB$_2$ bulks and strands are discussed. The influence of SiC, excess Mg, B4C, TiC, and their combination on Brr and Bc2 as distinct from connectivity and flux pinning is the focus of the work. SiC dopants increase Bc2 and Brr exhibit prominent, with little influence on connectivity or flux pinning. Excess Mg improves the transport current, changes the grain connectivity and lead to energy dissipation. We investigated the magnetic field behavior of MgB$_2$ thin films samples grown by in situ pulsed laser deposition and in situ reactive deposition technique on different substrates. We performed time-resolved magneto-optical imaging (TRMOI) measurements as a function of applied static field and for a static filed plus ac current to visualize the kinetic roughening of the flux penetration front. The TRMOI images are analyzed by employing dynamic scaling concepts used in the studies of interface roughening of stochastic systems. For both static field and ac current the resulting critical state shows self-affine structure characterized by universal exponents. [1] Dynamic scaling-laws determined in both cases are consistent with the directed percolation model, placing the vortex dynamics of MgB$_2$ in the same universality class as YBCO and Nb.

9:00AM U11.00006 Upper critical field study of MBE grown MgB$_2$ thin films, J. JAROSZYNSKI, F. HUNTE, A. GUREVICH, D.C. LARBALESTIER, Applied Superconductivity Center, NHMFL, Tallahassee, Y. ZHU, P.M. VOYLES, University of Wisconsin, Madison, Y. SHEN, R. GANDIKOTA, R. SINGH, J. ROWELL, N. NEWMAN, Arizona State University, Tempe — “Normal” alloying of MgB$_2$ enhances the electron scattering, as does radiation damage. As a result, the upper critical field Hc2($0$) parallel to the ab planes doubles from about 18 to 35 T. ASU has been growing films by non-equilibrium MBE methods and either intentionally doping with oxygen during growth, or by deposition at room temperature with subsequent annealing ex situ at rather low temperature: e.g. 350 °C for 36 hrs followed by 600 °C for 30 min. The resistive transitions of the films have been measured in fields up to 45 T at different temperatures. The measurements revealed strong enhancement of Hc2($0$). In particular, the cold-deposited film remains superconducting at 45 T at 5 K, while extrapolation yields Hc2($0$) higher than 65 T, almost as high as the best C-doped HPCVD films. At the same time, the film is strongly inhomogeneous, the resistivity is as high as 30 m$\Omega$cm, while the transitions are very broad, and the critical temperature is lowered to 24 K. However, dHc2/dT at Tc reaches a record high value of 2.7 T/K. These observations open up another way to get exceptional values in MgB$_2$ films.

9:12AM U11.00007 Novel properties in the normal state and the mixed state due to multiband effect in MgB$_2$, HAI-HU WEN, Institute of Physics, Chinese Academy of Sciences — Based on high quality MgB$_2$ thin films, we measured the longitudinal and transverse resistivity of seven different samples with variable disorders characterized by the residual resistivity ratio (RRR) ranging from 4.0 to 33.3. Strong nonlinear Hall effect and strong magneto-resistance have been found in clean samples and they decrease gradually with the increase of scattering centers or temperature. By fitting to the theoretical model for a four-band system, for the first time, we derived the scattering rates for each band. Non-trivial difference between the transport properties of these four bands are unraveled. In the mixed state, a non-vanishing dissipation has been observed in the low temperature regime. The Hall Effect measurement confirms that it is induced by the vortex motion. Together with the data of I-V curves, point-contact tunneling and the magnetization relaxation, we conclude that this non-vanishing dissipation in the zero temperature limit is induced by the proliferation of the pi-band quasiparticles, in association with the multigap feature. In collaboration with H. Yang, Y. Jia, J.R. Shi, L. Shan, C. Ren and Y.Z. Zhang at IOP, CAS and C.G. Zhuang, Z.K. Liu, Qi Li, Yi Cui, and X.X. Xi at Penn State University.
9:48AM U11.00008 Structural-Microstructural Characteristics and its Correlations with the Superconducting Properties of in-situ PIT Processed MgB\textsubscript{2} Tapes with Ethyltoluene and SiC Powder added, ANJANA ASTHANA, Superconducting Materials Center, National Institute for Materials Science, 1-2-1, Sengen, Tsukuba, Ibaraki, H. YAMADA, N. UCHIYAMA, Central Japan Railways Company, Oyama, Japan, A. MATSUMOTO, H. KITAGUCHI, Y. MATSU, H. KUMAKURA, Superconducting Materials Center, National Institute for Materials Science, 1-2-1, Sengen, Tsukuba, Ibaraki — The structure and microstructures of pure MgB\textsubscript{2}, ethyltoluene and ethyltoluene + SiC added MgB\textsubscript{2} tapes have been investigated by using selected area electron diffraction, bright field, dark field and high resolution electron microscopy. As reported, the Jc values of the ethyltoluene and ethyltoluene + SiC added MgB\textsubscript{2} tapes are much higher than the pure MgB\textsubscript{2} tape sample. Analysis of the microstructures shows that pure MgB\textsubscript{2} tape sample consist of grains of 100-200nm. With the addition of ethyltoluene and ethyltoluene + SiC to the starting powder of in situ processed MgB\textsubscript{2} tapes, the grain size decreases drastically to an average size of about 20-50nm. The higher Jc value of the ethyltoluene and ethyltoluene + SiC added MgB\textsubscript{2} tapes as compared to the pure MgB\textsubscript{2} tapes has been attributed to the decrease in grain size and better connectivity of the grains and presence of pinning centers as some precipitates and Mg\textsubscript{2}Si particles of size less than 100nm.

10:00AM U11.00009 Properties of MgB\textsubscript{2} Thin Films Grown at Different Temperatures by Hybrid Physical-Chemical Vapor Deposition\textsuperscript{1}, MENNO VELDHORST\textsuperscript{2}, KE CHEN, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania, USA, CHE-HUI LEE, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA, QI LI, XIAOXING XI, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania, USA — MgB\textsubscript{2} films grown by Hybrid Physical-Chemical Vapor Deposition (HPCVD) at high temperature excel in $\mathbf{T}_\mathbf{c}$ values as high as 20 K are obtained, comparable to the highest values observed for the A15 compounds. These studies thus allow an investigation of any known binary compound, but the $T_c$ values of elemental superconductors under extreme pressures are not far behind. We have recently used pressures as high as nearly 2 Mbar to induce superconductivity in Sc, Y, Lu, and CaLi\textsubscript{2}. In situ X-ray diffraction and atomic force microscopy show that the film is polycrystalline. The low-temperature grown MgB\textsubscript{2} films are promising as the top electrode for sandwich-type all-MgB\textsubscript{2} junctions to preserve the integrity of the barrier layer.

\textsuperscript{1}This work is supported by ONR.

\textsuperscript{2}Also with The Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

10:12AM U11.00010 Superconductivity in Sc, Y, Lu, and CaLi\textsubscript{2} under Extreme Pressures\textsuperscript{1}, M. DEBESSAIJ, J.J. HAMLIN, A.K. GANGOPADHYAY, J.S. SCHILLING, Dept. Physics, Washington U, St. Louis, MO, USA, T. MATSUOKA, K. SHIMIZU, KYOKUGEN, Osaka U, Japan — Following the first experiments by Sizoo and Onnes in 1925 on Sn, studies of superconductivity under high pressures have made important contributions by furthering our understanding of this exotic state and creating many new and novel superconducting materials, including O, Si, Fe, I, and Cs. Indeed, the number of elemental superconductors across the periodic table has almost doubled through the application of extreme pressures. MgB\textsubscript{2} exhibits the highest value of $T_c$ of any known binary compound, but the $T_c$ values of elemental superconductors under extreme pressures are not far behind. We have recently used pressures as high as nearly 2 Mbar to induce superconductivity in Sc, Y, and Lu, as well as to search for superconductivity in CaLi\textsubscript{2}. $T_c$ values as high as 20 K are obtained, comparable to the highest values observed for the A15 compounds. These studies thus allow an investigation into the question: what is the maximum possible value of $T_c$ in a phonon-mediated superconductor?

\textsuperscript{1}This research supported by NSF grant DMR-0703896.

10:24AM U11.00011 ABSTRACT WITHDRAWN

10:36AM U11.00012 Superconductivity in MgCNi\textsubscript{3}, Tunneling and heat capacity on single crystals\textsuperscript{1}, PETER SAMUELY, ZUZANA Pribulova, JOZEF KACMARCik, PAVOL SZABO, Centre of Low Temperature Physics at the IEP Slovak Academy of Sciences and P.J. Šafárík University, Watsonova 47, 040 01 Košice, Slovakia, CHRISTOPHE MARCENAT, CEA-Grenoble, Département de Recherche Fondamental sur la Matière Condensée, F-38054 Grenoble Cedex 9, France, THIERRY KLEIN, Institut Néel, CNRS, BP166 38042 Grenoble Cedex 9, France, D.-J. JANG, H.-G. LEE, H.-S. LEE, S.I. LEE, NVCRICS and Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea — MgCNi\textsubscript{3} reveals superconductivity despite a large molar volume of Ni atoms. The origin of superconductivity in this material has not yet been clarified. There is a lot of discrepancy in experimental results and physical interpretation where even unconventional pairing or a two-band model have been proposed for the system, but these suggestions are based on measurements on polycrystalline samples. Here we present the point-contact tunneling spectroscopy and ac-calorimetry measurements on single crystals of very good quality. Measurements have been performed in the temperature range from 0.7 K and in magnetic fields up to 8 T. The temperature dependence of the energy gap of the system is presented and compared to the BCS model.

\textsuperscript{1}This work has been supported by 6th FP EU grant No. MTKD-CT-2005-03002 and the Slovak Research and Development Agency contract No. LPP-0101-06.

10:48AM U11.00013 No Evidence for Spin Density Waves in Pb using Phonon Imaging\textsuperscript{1}, TIMOTHY HEAD\textsuperscript{2}, JAMES WOLFE, University of Illinois Urbana-Champaign — Phonon-imaging in superconducting Pb has proven to be a sensitive probe of quasiparticle density due to the highly anisotropic absorption of ballistic phonons by quasiparticles. Slower than expected temperature dependences of quasiparticle density observed previously by Wolfe and Short (Physica B 316, 107 (2002)) are explained here by taking into account the effects of nonequilibrium quasiparticles. Minimizing the effects of nonequilibrium quasiparticles enables us to extract a value of the zero-temperature superconducting gap parameter. We measure $\Delta = 1.32 \pm 0.07$ meV consistent with tunneling measurements in Pb and the conventional BCS picture, and inconsistent with earlier specific heat data that motivated the proposal of a spin-density wave ground state in Pb (Overhauser and Daemen, PRL 61, 1885 (1988)).

\textsuperscript{1}This work was supported by DOE grant DEFG02-96ER45439.

\textsuperscript{2}Now at Abilene Christian University

Thursday, March 13, 2008 8:00AM - 11:00AM — Session U12 DCMP: Strongly Correlated Electron Systems: Quantum Phase Transitions Morial Convention Center 203
8:00AM U12.00001 Quantum phase transition of a magnetic impurity in a dissipative environment¹, MENGXING CHENG, KEVIN INGERSENT, University of Florida, MATTHEW GLOSSOP, Rice University — We study the quantum phase transition (QPT) induced by dissipation in the Bose-Fermi Anderson model of a magnetic impurity that hybridizes with a metallic host and is also coupled (via its charge) to a bosonic bath having a spectral density proportional to $\omega^s$. For sub-Ohmic bath exponents $0 < s < 1$, numerical renormalization-group calculations show that upon increasing the coupling to the bosonic bath from zero, there is a crossover from a conventional (spin-sector) Kondo effect to a charge-Kondo effect. Further increase of the bosonic coupling results in a zero-temperature transition to a phase in which charge fluctuations on the impurity site are frozen out. Critical exponents describing the response of the impurity charge to a locally applied electric field are found to obey the hyperscaling relations characteristic of an interacting critical point. The numerical value of these exponents suggests that the QPT lies in the same universality class as that of the sub-Ohmic spin-boson model. Results for the Ohmic case $s = 1$ will also be presented.

¹Supported by NSF Grants DMR-0312939 and DMR-0710540.

8:12AM U12.00002 Quantum Criticality of the Pseudogapped Kondo Problem: Finite Temperature Scaling and Conformal Invariance, MATTHEW T. GLOSSOP, STEFAN KIRCHNER, QIMIAO SI, Department of Physics and Astronomy, Rice University — The critical destruction of the Kondo effect is of interest as a potential mechanism for quantum-critical heavy-fermion metals. Here, we study the pseudogapped Kondo model [1], with a conduction-electron density of states proportional to $\mid\tau\mid$, which provides a paradigm for understanding critical moment fluctuations. In general, an interacting quantum critical point (QCP), at a finite critical Kondo coupling $J_0$, separates Kondo-screened and free local-moment phases [2]. We focus on finite-$T$ scaling properties in the vicinity of the QCP, obtained using a dynamical large-N method for an SU(N) generalization of the model. Though the bulk lacks conformal invariance for $r > 0$, we show that correlation functions assume the form expected of a boundary conformal field theory, implying an enhanced symmetry at the QCP. We also address these and related issues in the N=2 model using a continuous-time quantum Monte Carlo impurity solver [3], which involves a stochastic evaluation of an expansion in the host-impurity hybridization. [1] D. Withoff and E. Fradkin, Phys. Rev. Lett. 64, 1835 (1990) [2] K. Ingersent and Q. Si., Phys. Rev. Lett. 89, 076403 (2002). [3] P. Werner et al., Phys. Rev. Lett. 97, 076405 (2006)

8:24AM U12.00003 Quantum-criticality in models of an impurity coupled to fermionic and bosonic baths¹, KEVIN INGERSENT, U. of Florida, MATTHEW GLOSSOP, Rice U. — Impurity models exhibiting quantum phase transitions (QPTs) have attracted interest in connection with impurities in cuprate superconductors, heavy-fermion quantum criticality, and quantum-dot devices. This talk focuses on three models describing an impurity level coupled both to a band of fermions (either spinful or spinless) with a density of states varying as $\mid\tau\mid$. However, for sufficiently strong fermionic pseudogaps (large values of $\tau$), new universality classes of QPT emerge.

¹Supported by NSF Grants DMR-0312939 and DMR-0710540.

8:36AM U12.00004 The Two-Impurity Anderson Model at Quantum Criticality¹, DAVID MROSS, Bonn University, Germany, HENRIK JOHANNESSON, Göteborg University, Sweden — We propose a realization of the two-impurity Anderson model in a double quantum-dot system. When charge transfer between the dots is suppressed the system exhibits a non-Fermi liquid critical line parameterized by the amount of charge localized on the dots. Employing conformal field theory techniques we identify the critical exponents that govern transport and thermodynamics in the vicinity of the critical line. We also determine the dynamical exponent that sets the time scale for buildup of the non-Fermi liquid state after the system is shifted into the critical region, e.g. by a sudden change of a nearby gate voltage.

¹Work supported by the Swedish Research Council

8:48AM U12.00005 ABSTRACT WITHDRAWN —

9:00AM U12.00006 Absence of quantum phase transition in two-state quantum dot¹, XIN WANG, ANDREW J. MILLIS, Columbia University — We use continuous-time quantum Monte Carlo methods to study a model of a spinless-fermion two state quantum dot which was argued in Ref. [1] to exhibit a quantum phase transition. We find instead a smooth behavior as parameters are varied. The generalization of the model to the spinful case is also presented. [1] D. I. Golosov and Y. Gefen, Phys. Rev. B 74, 205316 (2006).

¹This work was supported by the Nanoscale Science and Engineering Initiative of the National Science Foundation under NSF Award Number CHE-0615123 and by NSF-DMR-0705847

9:12AM U12.00007 Kondo destruction in the Bose-Fermi Kondo model with a singular dissipative spectrum: Exact solutions and their implications¹, JIANHUI DAI, Zhejiang University, C.J. BOLECH, QIMIAO SI, Rice University — Quantum dissipation induces a critical destruction of the Kondo screening, which is of interest in the contexts of quantum critical heavy fermions and magnetic mesoscopic structures. The sub-Ohmic Bose-Fermi Kondo (BFK) model provides a setting to study such an effect. Here, we show that this many-body problem is exactly solvable when the spectrum of the dissipative bosonic bath, $J(\omega)$, is singular, such that $J(\tau) = \text{const.}$. We determine the exact results for the local spin correlation functions, which imply that the singular longitudinal fluctuations of the bosonic bath play a dominant role. We also demonstrate how the large-N limit of an SU(N) generalization of the same model fails to capture the $N = 2$ physics in the cases of a singular dissipative bosonic spectrum, due to an interesting under-treatment of the longitudinal fluctuations. Our results resolve an apparent inconsistency between the previous results respectively found using numerical renormalization group and large-N treatments, providing evidence that the local quantum critical solution of the extended dynamical mean field approach to the Kondo lattice model indeed has a zero residual entropy.

¹J.D. has been partially supported by the NSF of China.

9:24AM U12.00008 ABSTRACT WITHDRAWN —
Quantum Criticality out of Equilibrium: Kondo Destruction and V/T Scaling in a Magnetic Single-Electron Transistor. STEFAN KIRCHNER, QIMIAO SI, Rice University — Non-equilibrium quantum phase transitions have so far received only limited attention despite the long-standing strong interest in classical out-of-equilibrium phase transitions. This is in part due to the fact that dynamics and statics are already intermixed at an equilibrium quantum phase transition. Nanostructured devices constitute simplified systems, both theoretically and experimentally, to study well-defined out-of-equilibrium states that give rise to unique steady-state limits. We recently showed that such a system, a magnetic single-electron transistor, can be tuned through a continuous quantum phase transition as the applied gate voltage is tuned [1,2]. The Kondo effect is critically destroyed across the quantum critical point, an effect that is also of interest in some bulk strongly correlated systems such as heavy fermions [3].


Current-Flow-Driven Nonequilibrium Paramagnetic-Ferromagnetic Phase Transitions. ADITI MITRA, New York University, IGOR ALEINER, ANDREW MILLIS, Columbia University — We study a 2d itinerant electron system near a ferromagnetic-paramagnetic quantum critical point, which has been driven out of equilibrium by current flow through its bulk. The lack of Galilean invariance in physically realistic models implies that there is no co-moving frame of reference where the physics is identical to that in the absence of current. In the vicinity of the equilibrium critical point the main effect of current flow is shown to be an effective temperature, with current induced drift giving subleading corrections. The current can also destabilize a classical order, and may give rise to new kinds of ordered or quasi-ordered phases.

Criticality in Inhomogeneous magnetic systems: Applications to Quantum Ferromagnets. R. SAHA, Dept. of Physics, Univ. of Oregon, Eugene, OR 97403 & Dept. of Physics, Univ. of Maryland, College Park, MD 20742, T. R. KIRKPATRICK, Dept. of Physics, Univ. of Maryland, College Park, MD 20742, D. BELITZ, Dept. of Physics, Univ. of Oregon, Eugene, OR 97403 — In standard phase transitions such as the liquid-gas transition, a homogeneous order parameter (OP) vanishes as one crosses from the ordered phase to the disordered one. An external field may preclude a macroscopic OP. This happens for a fluid in a gravitational field, where the transition becomes smeared [1] in the sense that the OP is nonzero everywhere, albeit very small in some regions of the phase diagram. A ferromagnet (FM) subject to mechanical stress is another realization of a system in an external field that has an inhomogeneous OP. We first investigate a classical Heisenberg FM, which is modeled by a $\phi^4$ theory with a spatially dependent mass $m(r)$. In contrast to the fluids case, we find a sharp phase transition where the envelope of the local magnetization vanishes uniformly, and mean-field critical exponents. The first order transition in quantum itinerant FMs also remains sharp and the fluctuation effects leading to a tricritical point are suppressed, and one recovers a quantum critical point with mean field exponents [2]. [1] J.V. Sengers and J.M.J. van Leeuwen, Physica A, 116, 345 (1982). [2] D. Belitz, T.R. Kirkpatrick, and R. Saha, Phys. Rev. Lett., 99, 147203(2007).

Non-Ginzburg-Landau Type Universality in Quantum Metamagnetism Induced by Topological Change of Fermi Surface: Applications to a Weak Itinerant-Electron Ferromagnet ZrZn$_2$. YOUEHI YAMAJI, TAKAHIRO MISAWA, Dept. of Applied Physics, Univ. Tokyo, MASATOSHI IMADA, Dept. of Applied Physics and JST-CREST, Univ. Tokyo — We clarify that metamagnetic transitions show unconventional properties as quantum phase transitions if they are accompanied by changes in Fermi-surface topology. Topological change of the Fermi surface makes the phase diagram qualitatively different from that of the conventional metamagnetic transitions; the quantum critical endpoint becomes not only the terminal of the finite-temperature critical line, but also the terminal of a quantum critical line of continuous Lifshitz transitions. Around the quantum critical terminal, power-law singularities of thermodynamic quantities are determined by the Fermi-surface topology and, therefore, are characterized neither by the Ising symmetry breaking nor by the Ginzburg-Landau-Wilson scheme proposed by Moriya, Hertz andMillis for the conventional quantum criticalities. We propose that such an unconventional universality indeed accounts for the metamagnetic transitions observed in ZrZn$_2$.

This work was supported by MEXT (Grand Nos. 17071003 and 16076212).

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This work was supported by National Science Foundation.
8:00AM U13.00001 Self-consistent van der Waals density functional: Development and Applications, VALENTINO COOPER, Rutgers University — The inability of density functional theory (DFT), with standard exchange-correlation functionals, to correctly describe van der Waals/Dispersion (vdW) interactions has severely limited its applicability to sparsely packed systems, such as organic and biological molecules. Numerous attempts have been made to correct these deficiencies; however, many of them either require extensive reparameterization for each new situation or scale poorly with system size. In this paper, I will discuss the development and implementation of an exchange-correlation functional which correctly incorporates non-local vdW interactions within DFT (vdW-DF). In addition, I will present our recent development of the corresponding exchange-correlation potential (Vxc). The Vxc gives us the ability to compute Hellmann-Feynman forces, allowing for structural relaxations and molecular dynamics simulation. Using the Vxc, I will examine the nature of the van der Waals bond between molecules. Finally, to demonstrate the power of the vdW-DF, I will discuss our relatively large-scale application of the functional to study the influence of stacking interactions on the structure and stability of DNA. Here, I will show how these interactions are crucial for defining the twist and base pair separation in DNA and how methyl-nucleobase and methyl-methyl interactions give additional stability to DNA.


8:36AM U13.00002 Stochastic Time-Dependent Current-Density Functional Theory, ROBERTO D’AGOSTA, University of California - San Diego — Static and dynamical density functional methods have been applied with a certain degree of success to a variety of closed quantum mechanical systems, i.e., systems that can be described via a Hamiltonian dynamics. However, the relevance of open quantum systems - those coupled to external environments, e.g., baths or reservoirs - cannot be overestimated. To investigate open quantum systems with DFT methods we have introduced a new theory, we have named Stochastic Time-Dependent Density Functional Theory (S-TDDFT) [1]: starting from a suitable description of the system dynamics via a stochastic Schrödinger equation [2], we have proven that given an initial quantum state and the coupling between the system and the environment, there is a one-to-one correspondence between the ensemble-averaged current density and the external vector potential applied to the system. In this talk, I will introduce the stochastic formalism needed for the description of open quantum systems, discuss in details the theorem of Stochastic TD-CDFT, and provide few examples of its applicability like the dissipative dynamics of excited systems, quantum-measurement theory and other applications relevant to charge and energy transport in nanoscale systems.


3Work supported by DOE grant DE-FG02-05ER46204

9:12AM U13.00003 Investigating interaction-induced chaos using time-dependent density functional theory, ADAM WASSERMAN, Harvard University — Systems whose underlying classical dynamics are chaotic exhibit signatures of the chaos in their quantum mechanics. In this talk I will discuss the possibility of using time-dependent density functional theory (TDDFT) to study the case when chaos is induced by electron interaction alone. Nearest-neighbor level- spacing statistics are in principle exactly and directly accessible from time-dependent density functional theory (TDDFT). Can the linear response formalism of TDDFT reveal the mechanism of chaos induced by electron-interaction alone? A simple model of a few-electron quantum dot highlights the necessity to go beyond the adiabatic approximation in TDDFT.

9:48AM U13.00004 Time-dependent NEGF calculations of extended systems, ALEXANDER PROCIUK, BARRY DUNIETZ, University of Michigan — A non-equilibrium GF (NEGF) model based on time dependent perturbation theory is developed to propagate electronic structure and molecular conductance of extended electrode-molecule-electrode nanostructures. In this model, we take advantage of the two time variable nature of the KB equations in order to formulate a mixed time-frequency representation for the lesser GF. This allows us to include bulk affected electrodes with non-trivial energy representations in our propagation. It also allows us to express dynamical observables such as current with highly informative Wigner distributions that shed light on the physical causes for certain dynamic features. Preliminary calculations, performed on simple systems, reveal that the dynamic current has both a direct and an alternating contribution. The direct current is due to a bulk affected state and the alternating component is due to a superposition of states. The amplitude of the alternating current can be changed dramatically by adjusting the bias pulse.

10:00AM U13.00005 Many-Body Density Matrix Perturbation Theory, C.J. TYMCGZAK, Texas Southern University — One fundamental limitation of quantum chemical methods is the accuracy of the approximate many-body theoretical framework that is utilized. Accurate many-body formalisms for quantum chemical methods do exist, but these methods are computationally very expensive. Methods also exist that are much less computationally expensive such as Hatree-Fock, Density Functional and the Hybrid Functional theories, but at a reduced representation of the exact many-body ground state. This severely limits their use to the system size. In the absence of an accurate representation of the many-body ground state. What is essential is a method which represents the many-body ground state accurately, but with a low computational cost. Recently, a method for determining the response, to any order of the perturbation, within the density matrix formalism has been discovered. This method is very simple and computationally efficient, and it immediately opens up the possibility of computing the variational many-body ground state to unprecedented accuracy within a simplified computational approach. Within this article, we report on the theoretical development of this methodology, which we refer to as Many Body Density Matrix Perturbation Theory. This theory has many significant advantages over existing methods. One, its computational cost is equivalent to Hartee-Fock. Two it is a variational upper bound to the exact energy. And three, it has no self-interaction.

10:12AM U13.00006 Conformational hierarchies of weakly bonded systems: Accuracy of dispersion corrected DFT, ALEXANDRE TKATCHENKO, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — It is well known that long-range dispersion interactions, important for stabilization of, e.g., molecular crystals, biomolecules and physisorption, are badly described by state-of-the-art xc functionals in DFT, but naturally included in post-HF methods or empirically in force field simulations. We have implemented a semi-empirical C6/R6 correction [1,2] in the numeric atom-centered orbital based code FHI-aims [3] and obtained correction parameters by fitting to a database of high quality ab initio calculations [2], improving on previous results due to the more accurate basis set (0.5 kcal/mol average error for binding energies using PBE0+P86). We assess the accuracy and impact of the correction on conformational energy hierarchies of (i) H2O6+ clusters (n=2-6), (ii) Al2 and Al2+, and (iii) infinite polyaniline conformers, comparing to published post-HF results for (i) and (ii). Even though the relative energies are not changed for small H2O clusters and Al2 compared to DFT-GGA, the impact of dispersion on the conformation hierarchy of larger systems is surprisingly large, reaching ~1-4 kcal/mol for different polyaniline conformers. [1] S. Grimme, J. Comput. Chem. 25, 1463 (2004) [2] P. Jurecka et al., J. Comput. Chem. 28, 555 (2007) [3] V. Blum et al., FHI ab initio molecular simulations (FHI-aims) project.

Thursday, March 13, 2008 8:00AM - 11:00AM
Session U13 DCOMP DCP: Focus Session: Frontiers in Electronic Structure Theory II
Morial Convention Center 204
10:24AM U13.00007 Iterative computation of dielectric eigenmodes, HUGH WILSON, FRANCOIS GYGI, GIULIA GALLI, University of California, Davis — We present an iterative method for the calculation of the eigenvectors of dielectric matrices of materials and nanostructures, based on Density Functional Theory, within a linear response framework. We show that by computing a relatively small number of eigenvectors via iterative dielectric response calculations, one may reconstruct the full dielectric matrix of a given system to high accuracy. The proposed method bypasses the need for the calculation of a large number of excited states required by earlier dielectric matrix computations based on the Random Phase Approximation. The scaling of the algorithm and the efficiency of the approach will be demonstrated by the calculation of the static dielectric properties of a variety of nanostructures, including silicon rods and slabs.

10:36AM U13.00008 Comparison of vibrational and electronic contributions to van der Waals interactions, MARK R. PEDERSON, Naval Research Laboratory, KYUNGWHWA PARK, Virginia Polytechnic Institute, AMY Y. LIU, Georgetown University — The van der Waals interaction can be caused by either ionic vibrations or instantaneous electronic motion relative to the atomic center. In this study, the vibrational contribution to the van der Waals interaction is formulated by considering the interaction between induced dipoles caused by the infrared-active normal modes of a neutral molecule. Using the derived formula, the contribution is quantified, within the density-functional theory formalism, using a screened, i.e., self-consistent, vibrational polarization. Applications for several neutral nonpolar dimers are presented. It is found that the vibrational contributions for the dimers are substantially smaller than their electronic contributions. The ratio of the vibrational to electronic contributions depends strongly on the ratio of the screened vibrational to electronic polarizabilities and on the ratio of the frequency of the strongest infrared-active mode to an ionization energy.

10:48AM U13.00009 Recent progress in ab initio density matrix renormalization group methodology, JOHANNES HACHMANN, JONATHAN J. DORANDO, GARNET KIN-LIC CHAN, Cornell University — We present some recent developments in the ab initio density matrix renormalization group (DMRG) method for quantum chemical problems, in particular our local, quadratic scaling algorithm [1] for low dimensional systems. This method is particularly suited for the description of strong nondynamic correlation, and allows us to compute numerically exact (FCI) correlated energies for large active spaces, up to one order of magnitude larger than can be done by conventional CASCI techniques. Other features of this method are its inherent multireference nature, compactness, variational results, size-consistency and size-extensivity. In addition we will review the problems (predominantly organic electronic materials) on which we applied the ab initio DMRG: 1) metal-insulator transition in hydrogen chains [1] 2) all-trans polyacetylene [1] 3) acenes [2] 4) polydiacetylenes [3]. References [1] Hachmann, Cardeno, Chan, JCP 125 (2006), 144101. [2] 

Thursday, March 13, 2008 8:00AM - 11:00AM — Session U14 DAMOP: Focus Session: Exotic Phases in Ultracold Fermi Gases Morial Convention Center 205

8:00AM U14.00001 FFLO states in resonant Fermi gases, SUNKGIT YIP, Academia Sinica, Taiwan — We discuss the possible phases of two-component Fermi gas with population imbalance. In particular, we consider the various states proposed by Fulde-Ferrell and Larkin-Ovchinnikov. We distinguish between the plane-wave state Delta ~ e^{i\eta}, where the magnitude of the order parameter is uniform in space but the phase varies continuously in space, from those where the order parameters are real but change sign from one spatial region to the other. The later states, considered first by Larkin and Ovchinnikov, occupy a much larger region in the uniform phase diagram than previously suggested by other authors. If time permits, we shall discuss also the situation in a harmonic trap.

8:36AM U14.00002 Is There an FFLO Region in a Polarized Trapped Unitary Fermi Gas?, WILLIAM SCHNEIDER, The Ohio State University, RAJDEEP SENSARMA, Harvard University, ROBERTO DIENER, MOHIT RANDERIA, The Ohio State University — We have studied strongly interacting polarized gases in a harmonic trap beyond the local density (LDA) approximation using the Bogoliubov-deGennes equations. In particular, we are interested in the region separating an unpolarized superfluid core in the center and a fully polarized majority gas in the intermediate lattice limit, where the anisotropy in the atomic motion enhances Fermi surface 'nesting', but there is still a small amount of tunneling between tubes to provide long-range order. Finally we discuss the spatial arrangement of phases in a trap: in 3D the homogenous superfluid phase sits in the center of the trap, while in 1D it lies on the edge. We explain how this pattern evolves as one changes the lattice intensity.

8:48AM U14.00003 Polarized Fermi superfluids between one and three dimensions, MEERA PARISH, Princeton University, STEFAN BAUR, ERICH MUELLER, Cornell University, DAVID HUSE, Princeton University — We theoretically explore the phase diagram of a polarized two-component Fermi gas divided into an array of tubes by a two-dimensional optical lattice. By increasing the intensity of the optical lattice one suppresses the inter-tube hopping, and one can drive a crossover from three to one-dimensional behavior. We show that the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) inhomogeneous superfluid phase is stabilized by the lattice, and we argue that the most promising parameters for observing the FFLO phase are in the intermediate lattice limit, where the anisotropy in the atomic motion enhances Fermi surface 'nesting', but there is still a small amount of tunneling between the tubes to provide long-range order. Finally we discuss the spatial arrangement of phases in a trap: in 3D the homogeneous superfluid phase sits in the center of the trap, while in 1D it lies on the edge. We explain how this pattern evolves as one changes the lattice intensity.

9:00AM U14.00004 Dimensional crossover from Quasi-1D to 3D in spin-polarized Fermi superfluids, STEFAN BAUR, Cornell University, MEERA PARISH, Princeton University, ERICH MUELLER, Cornell University, DAVID HUSE, Princeton University — We use a zero temperature Bogoliubov de Gennes mean field theory to study the evolution of the exotic FFLO superfluid in a spin-imbalanced Fermi gas as one progresses from quasi-1D to 3D by changing the coupling between an array of tubes. The boundary between the uniform BCS superfluid and the FFLO state is determined by examining the energetics of a single π-domain wall in the superfluid order parameter. In the quasi-1D limit, each tube contains a single excess particle at the center of each domain wall and the spectrum of single particle excitations is gapped. As one approaches 3D there is a phase transition where this commensurability condition is relaxed and gapless single particle excitations can be found. [1] M. M. Parish, S. K. Baur, E. J. Mueller, and D. A. Huse, arXiv:0709.1120

1This work was supported in part by the Army Research Office Grant No. W911NF-07-1-0464.
10:00AM U14.00009 P-wave Pairing in Two-Component Fermi System with Unequal Population near Feshbach Resonance.1 RENYUAN LIAO, FLORENTIN POPESCU, KHANDKER QUADER, Kent State University — We explore p-wave pairing in a single-channel two-component Fermi system with unequal population near Feshbach resonance. Our analytical and numerical study reveal a rich superfluid (SF) ground state structure as a function of imbalance. In addition to the state $\Delta_{k\uparrow} \propto Y_{l\downarrow}, a$ multitude of “mixed” SF states formed of linear combinations of $Y_{l\downarrow}$’s give global energy minimum under a phase stability condition; these states exhibit variation in energy with the relative phase between the constituent gap amplitudes. States with local energy minimum are also obtained. We provide a geometric representation of the states. A $T=0$ polarization vs. p-wave coupling phase diagram is constructed across the BEC-BCS regimes. With increased polarization, the global minimum SF state may undergo a quantum phase transition to the local minimum SF state.

1This work is partially supported by funding from ICAM.

10:12AM U14.00010 P-wave Paired Ground state Structure of Two-component Population Imbalanced Fermi Systems with Unequal Mass1. FLORENTIN POPESCU, RENYUAN LIAO, KHANDKER QUADER, Kent State University — Effects of unequal mass on p-wave pairing in population imbalanced two-component Fermi systems is studied using a single-channel fermionic Hamiltonian. Provided certain phase criteria are satisfied among the orbital gap parameters, a rich structure of the ground state is obtained. The global and local minima ground state energies are determined analytically. By numerically solving the gap and number equations, we construct $T=0$ polarization vs. p-wave coupling phase diagram across the BEC-BCS regime for different mass ratios. This shows the existence of two superfluid phases, SF1 is enhanced; SF2 is not significantly affected. Competition between mass ratio and polarization is studied; the superfluid transition temperature shows interesting behavior versus the mass ratio at high polarizations. At large polarizations, a stable p-wave superfluid would survive only for small mass ratios, and for mass ratios close to unity.

1The work is partially supported by funding from ICAM.

10:24AM U14.00011 Orbital ordering in an atomic Mott insulator of p-band fermions. ERHAI ZHAO, W. VINCENT LIU, University of Pittsburgh — We derive the low energy effective model describing the orbital degrees of freedom of strongly interacting spinless p-orbital fermionic atoms in 2D optical lattices. Virtual hopping processes of $p_x$ and $p_y$ fermions give rise to direct and multi-particle orbital exchanges in the strong coupling regime. For the square lattice, we show that the effective orbital Hamiltonian is equivalent to a quantum spin-1/2 XXZ model. In the limit where the transverse hopping is much smaller than the longitudinal hopping, the XXZ model reduces to an antiferromagnetic Ising model. Thus the atomic Mott insulator is antiferro-orbitally ordered. We also present results for other simple 2D lattices and discuss the experimental signatures of various orbital orderings.
10:36AM U14.00012 Density waves and superconductivity in rapidly rotating atomic Fermi gases. GUNNAR MOLLE, NIGEL R. COOPER, University of Cambridge — We study theoretically the low-temperature phases of a two-component atomic Fermi gas with attractive s-wave interactions under conditions of rapid rotation [1], a problem related to the discussion of high-field superconductivity in the solid state [2]. The regime of interest for atomic gases differs substantially from solid state conditions: the rotation does not lead to any Zeeman splitting which might suppress high-field SC order; the short-range interactions allow density wave order to develop (contrary to long-range Coulomb interactions). We show that the low-temperature phases of an atomic Fermi gas with attractive interactions involve an interesting interplay between CDW and superconducting phases. In the extreme quantum limit, when only the lowest Landau level is occupied, we employ a renormalization group approach [3] to show that the system is unstable to CDW order along the rotation axis. At lower rotation rates, we show how CDW and SC can coexist, leading to supersolid behaviour.


10:48AM U14.00013 Quantum Hall Transition near a Feshbach Resonance in Fast Rotating Fermi Gases1, KUN YANG, National High Magnetic Field Lab and Florida State University, HUI ZHAI, UC Berkeley and Lawrence Berkeley Lab — We consider two-species of fermions in a rotating trap that interact via an s-wave Feshbach resonance, at total Landau level filling factor two (or one for each species). We show that the system undergoes a quantum phase transition from a fermion integer quantum Hall state to a boson fractional quantum Hall state as the pairing interaction strength increases, with the transition occurring near the resonance. The effective field theory for the transition is shown to be that of a (emergent) massless relativistic bosonic field coupled to a Chern-Simons gauge field, with the coupling giving rise to semionic statistics to the emergent particles.

1Reference: arXiv:0709.2934

Thursday, March 13, 2008 8:00AM - 11:00AM –
Session U15 GQI: Focus Session: Open Quantum Systems and Decoherence
Morial Convention Center 207

8:00AM U15.00001 Coherence and control of single electron spins in quantum dots1, LIEVEN VANDERSYPEN, Kavli Institute NanoScience TU Delft — Following our earlier work on single-shot read-out and relaxation of a single spin in a quantum dot, we now demonstrate coherent control of a single spin (detection is done using a second spin in a neighbouring dot). First, we manipulate the spin using conventional magnetic resonance. Next, we show that we can also rotate the spin using electric fields instead of magnetic fields. In both cases, 90 rotations can be realized in about 50 ns or less. We use these control techniques to probe decoherence of an isolated electron spin. The spin dephases in about 30 ns, due to the hyperfine interaction with the uncontrolled nuclear spin bath in the host material of the dot. However, since the nuclear spin dynamics is very slow, this dephasing can be largely reversed using a spin-echo pulse. Echo decay times of about 0.5 us are obtained at 70 mT. In parallel, we have started work on quantum dots in graphene, which is expected to offer superior coherence times. As a first step, we have succeeded in opening a bandgap in bilayer graphene, necessary for electrostatic confinement of carriers.
F.H.L. Koppens et al., arXiv:0711.0479.
J.B. Oostinga, Nature Mat., in press.

1Supported by NWO and FOM.

8:36AM U15.00002 Non-Markovian thermalization for a few qubit system, PEDER MANRIQUE, FERNEY RODRIGUEZ, Universidad de los Andes — Non-Markovian dynamics in the thermalization process of a single and coupled-qubit systems are analyzed by means on an effective master equation. Memory effects are included in a time dependent relaxation constant which is obtained from a proper bosonic bath spectral function. For different initial states, the population and coherence are studied as a function of the qubit-bath coupling strengths and bath temperature. Clear signatures of non-exponential decays for the qubit density matrix elements are found in a short-time regime corresponding to the back action of the qubit system on the bath dynamics. In the case of realistic two-qubit systems, such as quantum dots, entanglement oscillations should be observable.

8:48AM U15.00003 Decoherence of coupled electron spins via nuclear spin dynamics in quantum dots1, WEN YANG, REN-BAO LIU, Department of Physics, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong, China — Decoherence of coupled electron spins due to electron-nuclear hyperfine interaction in double quantum dots is a major issue of solid-state quantum computation. Using an interacting nuclear spin bath model, we show theoretically that the exchange interaction between the two electron spins renormalizes the pair- flip excitation energy in the bath and modifies the non- Markovian bath dynamics, which in turn changes the electron singlet-triplet (S-T) decoherence arising from electron-nuclear entanglement. As the energy renormalization varies with the Overhauser field mismatch between the quantum dots, the S-T decoherence depends on the sampling of nuclear spin states from an ensemble, leading to the transition from super-exponential decoherence in single-sample dynamics to power-law decay under ensemble average,[1] in contrast with the sample-independent super-exponential decoherence of a single electron spin in one dot.

1This work was supported by Hong Kong RGC Project 2160285.

9:00AM U15.00004 Rabi oscillations decay from interaction with dynamical spin environments1, V.V. DOBROVITSKI, Ames Laboratory and Iowa State University, Ames, IA 50011, A.E. FEIGUIN, University of Maryland, College Park, MD 20742, and Microsoft Station Q, University of California, Santa Barbara, CA 93106 — Studying decoherence of spins/qubits interacting with a spin bath is important for quantum computation, high-precision metrology, coherent spintronics. Measurements of the Rabi oscillations decay provide much information about the decoherence dynamics and properties of the spin in single-spin quantum dots, dopant spins in a solid-state matrix, etc. [1] Also, for a static bath, application of a large Rabi field suppresses decoherence, changing fast exponential decay into slow power-law one. [1] However, internal dynamics of spin environment is important in such systems as NV centers in diamonds, magnetic molecules, and rare-earth dopant spins in solid state, but decay of Rabi oscillations for dynamical spin bath has been little studied. We present a detailed theoretical investigation of Rabi oscillations decay for a spin bath dynamical system, demonstrating new unusual decay regimes useful for characterization of the bath and decoherence suppression.


1Supported by DOE, NSF, AFOSR.
The paths difference, together with a phase rigidity. The solution shows that the interference visibility has a lobe pattern with applied bias with a period proportional to the average path length (and independent of the non-interacting Hamiltonian. It causes correlations inside each of the two MZI arm, resulting in the electrons affecting each other’s phase. An approximate difference. We argue that these effects have a fundamental reason. A simple invariance argument leads to an additional interaction term that must be added to interference visibility showed an unexplained lobe pattern behavior with a peculiar phase rigidity. Moreover, the effect did not depend on the MZI paths theoretically the behavior of the current oscillations in an electronic Mach-Zehnder interferometer (MZI) as a function of its source bias. Recently, The MZI has been shown to exhibit periodic oscillations in the output current as the source bias is varied. These oscillations are due to quantum interference effects and are of fundamental importance in quantum computing and quantum information processing.

We acknowledge support from NSF (DMR-0304380) and NSA, through the Laboratory of Physical Sciences.

Boundary Conditions for Open Rotating Quantum Systems, ARTHUR DAVIDSON, Carnegie Mellon University, ECE Dept, Pittsburgh PA 15213 — The customary boundary conditions for a 1D rotational system (e.g. a rigid rotor on a surface) are continuity of the complex wave function and its gradient. These four boundary conditions are sufficient if the potential energy satisfies rotational symmetry, but fall for non-rotational potentials. However, classical systems with a rotational coordinate and non-rotational potential are easily solved if the gradient of the potential, the force, is rotational. A solution is thus required for Schroedinger’s equation with a rotational coordinate and force, but non-rotational potential. Such solutions exist only in some spherical coordinate systems. However, the non-rotational potential will lead to non-rotational solutions which will not be rotational. It will be shown that the modified boundary conditions are continuity of three real quantities: the probability density, the gradient of the probability density, and the probability current density. Moreover, with these boundary conditions and non-rotational potential, energy can flow both ways between the system and its environment. The discontinuous wave functions obey the new boundary conditions, but nonetheless are not generally superposable. A subset of the discontinuous wave functions can be superposed, however, yielding the usual result for angular momentum states. The non-supersposable wave functions offer an alternate interpretation of the Schroedinger’s cat paradox.

Non-Markovian Open Quantum Systems, CESAR RODRIGUEZ-ROSARIO, E.C.G. SUDBAN, The University of Texas at Austin — A generalized non-markovian master equation is derived from the dynamical map of systems initially correlated with their environment. We study the connection between the initial correlations and the non-markovian memory effects. The significance of not-complete positive maps in order to obtain a consistent theory of non-markovian quantum dynamics is discussed. Previous specific instances of non-markovian master equations are examined in this framework.

Finite representations of continuum environments, MICHAEL ZWOLAK, Los Alamos National Laboratory — Understanding dissipative and decohering processes is fundamental to the study of non-equilibrium systems and quantum computing, and such processes can even induce quantum phase transitions. A typical construction is to have a system connected to a continuum environment, which acts as the source of dissipation or decoherence, or as a reservoir of particles. If the connection is strong or the environment has long-range correlations in time, the system dynamics are not easily separated from the dynamics of the environment. To study this situation numerically, one option is to simulate both the system and environment. This is a viable option so long as an efficient finite representation of the environment can be constructed. We will discuss a procedure to construct finite representations based on the concept of two-site recurrence and increasing smoothness. For solvable cases of non-interacting bosons, the procedure gives an exponential reduction in the number of discrete modes necessary to achieve some given accuracy in a real-time simulation. We will also discuss application of this procedure to interacting systems.

Induced decoherence and entanglement by an interacting spin chain, POCHUNG CHEN, Nat’l Tsing-Hua Univ, Hsinchu, CHENG-YAN LAI, JO-TZU HUNG, CHUNG-YU MOU — We study the reduced dynamics of a single or two qubits coupled to an interacting spin chain using time-dependent density matrix renormalization group (TD-DMRG) technology. By using TD-DMRG we can go beyond the uniform coupling central spin model and evaluate nonperturbatively the reduced dynamics even when the coupling between qubits and the chain is non-uniform. Furthermore, the qubit-bath interaction can be of Ising, XY, or Heisenberg type. This allows us to go beyond pure dephasing model. For single qubit we use Loschmidt echo to gauge the decoherence and investigate how the short time decay parameter and large time behavior are linked to the phase of spin chain. We use concurrence to quantify the (dis)-entanglement process of two qubits due to spin chain. We show that one can induced entanglement for an initially disentangled pair of qubit. The competition between induced decoherence and entanglement is discussed.

Temperature Exchange in a System of Two Harmonic Oscillators, ANTONIA CHIMONIDOU, GEORGE SUDARSHAN, University of Texas at Austin — We study the process by which quantum correlations are created when an interaction Hamiltonian is repeatedly applied to a system of two harmonic oscillators for some characteristic time interval, under what we call the “interact-refresh-repeat” scheme. We show, for example, that the oscillator frequencies are equal, the initial Maxwell-Boltzmann distributions of the uncoupled parts evolve to a new Maxwell-Boltzmann distribution that is not rotationally symmetric. Furthermore, we discuss why the equilibrium reached when the two oscillator frequencies are unequal, is not a thermal one. More specifically, we show that the ratio of the harmonic oscillator temperatures at the new equilibrium state is completely determined by the ratio of the inverse harmonic oscillator frequencies. We conclude that the selection rules imposed by the interaction Hamiltonian override the expected statistical mechanical effects. All the calculations are exact and the results are obtained through an iterative process, without using perturbation theory.

Impact of classical forces and decoherence in three-terminal Aharonov-Bohm devices, ELIA STRAMBINI, VINCENTO PIAZZA, FABIO BELTRAM, NEST INFN-CNR & Scuola Normale Superiore, I-56126 Pisa, Italy, GIOVANNI BIASIOL, Laboratorio Nazionale TASC INFN-CNR, I-34012 Trieste, Italy, LUCIA SORBIA, NEST INFN-CNR & Scuola Normale Superiore, I-56126 Pisa, Italy & Laboratorio Nazionale TASC INFN-CNR, I-34012 Trieste, Italy — Multi-terminal Aharonov-Bohm (AB) rings are ideal building blocks for quantum networks (QNs) thanks to their ability to transform input states into controlled coherent superpositions of output states. We report on experiments performed on three-terminal GaAs/AlGaAs AB devices and compare our results with a scattering-matrix model of our device including Lorentz forces and decoherence. Our devices were studied as a function of external magnetic field (B) and gate voltage (V g) down to a T=350 mK. The total output current from two terminals while applying a small bias to the third lead was found to be symmetric with respect to B with clear AB oscillations showing abrupt phase jumps between 0 and 2g differing due to the Lorentz force. Surprisingly, the individual outputs show an almost linear dependence of the oscillation phase on the external electric field. We emphasize that a simple scattering-matrix approach does not explain the observed behavior and show how to extend this model in order to fully describe the observed phenomena.

The Behavior of Electronic Interferometers in the Non-Linear Regime, IZHAR NEDER, ERAN GINOSSAR, Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76000, Israel — We investigate theoretically the behavior of the current oscillations in an electronic Mach-Zehnder interferometer (MZI) as a function of its source bias. Recently, the MZI interference visibility showed an unexplained lobe pattern behavior with a peculiar phase rigidity. Moreover, the effect did not depend on the MZI paths difference. We argue that these effects have a fundamental reason. A simple invariance argument leads to an additional interaction term that must be added to the non-interacting Hamiltonian. It causes correlations inside each of the two MZI arm, resulting in the electrons affecting each other’s phase. An approximate solution shows that the interference visibility has a lobe pattern with applied bias with a period proportional to the average path length (and independent of the paths difference), together with a phase rigidity.
10:48AM U15.00013 What is quantum about quantum trajectory equations?, JAY GAMBITTA, Institute of Quantum Computing, HOWARD WISEMAN, STÈVE JONES, ERIC CAVALCANTI, Griffith University — Quantum trajectory equations are stochastic equations for the state of an open quantum system conditioned on a monitoring i.e. a continuous-in-time measurement of a bath to which it is coupled. They are closely related to classical stochastic equations for classical probability distributions called filtering equations (e.g. the Kalman filter). Given this close relation, the question arises: what is quantum about quantum trajectory equations? In this talk I suggest that the answer lies in the ability of an experimenter to choose different monitoring schemes. Moreover, I propose that there is an experimental way to distinguish between cases where this choice does demonstrate the quantum nature of the noise, and the cases where it does not.

Thursday, March 13, 2008 8:00AM - 10:36AM —
Session U16 DBP: Focus Session: Medical Physics and Radiation Biology
Morial Convention Center

8:00AM U16.00001 Image-Guided Radiation Therapy: the potential for imaging science research to improve cancer treatment outcomes1, JEFFREY WILLIAMSON2, Virginia Commonwealth University — The role of medical imaging in the planning and delivery of radiation therapy (RT) is rapidly expanding. This is being driven by two developments: image-guided radiation therapy (IGRT) and biological image-based planning (BIBP). IGRT is the systematic use of serial treatment-position imaging to improve geometric targeting accuracy and/or refine target definition. The enabling technology is the integration of high-performance three-dimensional (3D) imaging systems, e.g., onboard kilovoltage x-ray cone-beam CT, into RT delivery systems. IGRT seeks to adapt the patient’s treatment to weekly, daily, or even real-time changes in organ position and shape. BIBP uses non-anatomic imaging (PET, MR spectroscopy, functional MR, etc.) to visualize abnormal tissue biology (angiogenesis, proliferation, metabolism, etc.) leading to more accurate clinical target volume (CTV) delineation and more accurate targeting of high doses to tissue with the highest tumor cell burden. In both cases, the goal is to reduce both systematic and random tissue localization errors (2-5 mm for conventional RT) conformity so that planning target volume (PTV) margins (varying from 8 to 20 mm in conventional RT) used to ensure target volume coverage in the presence of geometric error, can be substantially reduced. Reduced PTV expansion allows more conformal treatment of the target volume, increased avoidance of normal tissue and potential for safe delivery of more aggressive dose regimens. This presentation will focus on the imaging science challenges posed by the IGRT and BIBP. These include: Development of robust and accurate nonrigid image-registration (NIR) tools: Extracting locally nonlinear mappings that relate, voxel-by-voxel, one 3D anatomic representation of the patient to differently deformed anatomies acquired at different time points, is essential if IGRT is to move beyond simple translational treatment plan adaptations. NIR is needed to map segmented and labeled anatomy from the pretreatment planning images to each daily treatment position image and to deformably map delivered dose distributions computed on each time instance of deformed anatomy, back to the reference 3D anatomy. Because biological imaging must be performed offline, NIR is needed to deformably map these images onto CT images acquired during treatment. Reducing target and organ contouring errors: As IGRT significantly reduces impact of differences between planning and treatment anatomy, RT targeting accuracy becomes increasingly dominated by the remaining systematic treatment-preparation errors, chiefly error in delineating the clinical target volume (CTV) and organs-at-risk. These delineation errors range from 1 mm to 5 mm. No single solution to this problem exists. For BIBP, a better understanding of tumor cell density vs. signal intensity is required. For anatomic CT imaging, improved image reconstruction techniques that improve contrast-to-noise ratio, reduce artifacts due to limited projection data, and incorporate prior information are promising. More sophisticated alternatives to the current concept fixed boundary anatomic structures are needed, e.g., probabilistic CTV representations that incorporate delineation uncertainties. Quantifying four-dimensional (4D) anatomy: For adaptive treatment planning to produce an optimal time sequence of delivery parameters, a 4D anatomic representation, the spatial trajectory through time of each tissue voxel, is needed. One approach is to use sequences of deformation vector fields derived by non-rigidly registering each treatment image to the reference planning CT. One problem to be solved is prediction of future deformed anatomies from past behavior so that time delays inherent in any adaptive replanning feedback loop can be overcome. Another unsolved problem is quantification 4D anatomy uncertainties and how to incorporate such uncertainties into the treatment planning process to avoid geometric ‘miss’ of the target tissue.

1Supported by grant P01 CA116602 awarded by the National Institutes of Health
2Richmond, VA

8:36AM U16.00002 Bridging the Gaps between IGRT Systems and R&V Systems, YULONG YAN, XUEJUN WENG, JOSE PENAGARICANO, VANÉERAT RATAÑATHARATHORN, University of Arkansas for Medical Sciences — Image Guided Radiation Therapy (IGRT) is the next-generation of technology for high precision radiotherapy. BrainLAB ExacTrac and Tomotherapy are two of them. Unfortunately, neither of the two communicates with any Record and Verify (R&V) system for seamless radiation therapy workflow. So two dedicated software systems, iPump and ScreenBee, have been developed respectively to bridge the gaps between IGRT systems and the R&V systems to allow remote image reviewing as well as paperless future. Both iPump and ScreenBee have been extensively tested and evaluated in our clinic. They reduce the cost and improve the efficiency and the safety of clinical procedures. They also act as key integral components of our facility on its way toward the digital and paperless future.

8:48AM U16.00003 Hyperthermal heavy ion damage to DNA bases1, SARVENAZ SARABIPOUR, ZONGWU DENG, MICHAEL HUELS, Ion Reaction Laboratory, Dep. of Nuclear Medicine & Radiobiology, Univ. of Sherbrooke, QC, Canada — Ionization and fragmentation of DNA is a key step in biological radiation damage. When heavy ions cross the cell, secondary ballistic ions, electrons and radicals are generated along the ion tracks. Here we report measurements of ionic fragments induced by 1-100eV Ar$^+$ irradiation of Adenine, Guanine and Cytosine films on Pt. Experiments are conducted with a UHV ion-beam apparatus consisting of a low energy ion source, a beam line with high resolution magnetic mass spectrometer (MS), a biomolecular film preparation system, and a reaction chamber with high-resolution quadrupole MS to monitor desorbing ion yields. Among the major fragments, NH$_2^+$ was identified in the desorption mass spectra of all bases examined, indicating efficient de-amination; in cells this results in pre-mutagenic lesions. Several important factors, e.g. intra/inter-molecular proton/hydrogen tunneling, tautomeric equilibrium and the molecular geometry of the bases in the films likely contribute to ion induced de-amination, and will be discussed here.

1Funded by NSERC & CSA.
9:00AM U16.00004 Physical and Clinical Evaluation of Standardized uptake values
Cristina Lois, University of Tennessee, Knoxville, TN, Bjoern W. Jakoby, University of Surrey, Guildford, UK, Karl Hubner, University of Tennessee, Knoxville, TN, Mario Canadas, CIEMAT, Madrid, Spain, David W. Townsend, University of Tennessee, Knoxville, TN — The Standardized Uptake Value (SUV) is often used in postion emission tomography (PET) to differentiate malignant from benign tumors, and to monitor the progress of the patient’s response to therapy. Despite its name, SUV may depend on both PET scanner hardware and software details, and will depend on the imaging protocol. In this paper, we present a study of the SUV variability according to these external factors. To study the influence of the PET device, phantom studies were performed on two different PET/CT scanners. SUVs were obtained using several reconstruction algorithms and different reconstruction matrix sizes. To study the influence of the imaging protocol, patients were injected with 370 MBq of 18F-FDG and scanned at 60 and 90 min post-injection. SUVs were obtained applying several clinical image reconstruction algorithms. Significant differences in SUVs were obtained depending on the PET scanner, reconstruction method, and imaging protocol. It is essential, therefore, to follow a strict protocol in order to reliably compare FDG uptake with SUVs. Our results may have a significant clinical impact in order to provide an unbiased SUV threshold to determine malignancy.

9:12AM U16.00005 The Dose Response Relationship for Radiation Carcinogenesis
Eric Hall, Columbia University — Recent surveys show that the collective population radiation dose from medical procedures in the U.S. has increased by 750% in the past two decades. It would be impossible to imagine the practice of medicine today without diagnostic and therapeutic radiology, but nevertheless the widespread and rapidly increasing use of a modality which is a known human carcinogen is a cause for concern. To assess the magnitude of the problem it is necessary to establish the shape of the dose response relationship for radiation carcinogenesis. Information on radiation carcinogenesis comes from the A-bomb survivors, from occupationally exposed individuals and from radiotherapy patients. The A-bomb survivor data indicates a linear relationship between dose and the risk of solid cancers up to a dose of about 2.5 Sv. The lowest dose at which there is a significant excess cancer risk is debatable, but it would appear to be between 40 and 100 mSv. Data from the occupation exposure of nuclear workers shows an excess cancer risk at an average dose of 19.4 mSv. At the other end of the dose scale, data on second cancers in radiotherapy patients indicates that cancer risk does not continue to rise as a linear function of dose, but tends towards a plateau of 40 to 60 Gy, delivered in a fractionated regime. These data can be used to estimate the impact of diagnostic radiology at the low dose end of the dose response relationship, and the impact of new radiotherapy modalities at the high end of the dose response relationship. In the case of diagnostic radiology about 90% of the collective population dose comes from procedures (primarily CT scans) which involve doses at which there is credible evidence of an excess cancer incidence. While the risk to the individual is small and justified in a symptomatic patient, the same is not true of some screening procedures is asymptomatic individuals, and in any case the huge number of procedures must add up to a potential public health problem. In the case of radiation oncology, modern innovations such as Intensity Modulated Radiation Oncology or Proton Therapy both result in a substantial total-body dose to the patient, which must result in an increased incidence of second cancers. The technology exists to reduce these total body doses and the problem needs to be addressed.

9:48AM U16.00006 Panel Discussion on Medical Physics and Radiation Biology and pathways to these fields
Paul Gueye, Hampton University — Medical Physics is one of the less know physics field but one that has the most impact on our daily life. It is intrinsically linked to radiation biology as the latter provides crucial inputs to the former including treatment planning software packages, understanding of cancer treatment optimization, etc. This panel discussion, composed of renown experts in these fields and who are part of the four medical physics sessions to be presented during this 2008 APS March meeting, will provide an environment for the audience to fully understand what medical physics and radiation biology are about and the various pathways to become a successful practitioner or researcher for contributing in these fields.

10:24AM U16.00007 Anomalous Effect of Surface Diffusion on NMR Signal in Restricted Geometry
Neranjani Edirisinghe, Vadym Apalkov, Gennady Cymbalyuk, Georgia State University — The diffusion of magnetic molecules along the surface of restricted media and the coupling on the surface will strongly modify the echo attenuation NMR signal in the pulse field gradient measurements. The origin of this strong effect is the change of the symmetry of the lowest diffusion eigenmode of the system. We illustrate the effect of surface diffusion for cylindrical symmetric system. We find the parameters of the system under which the anomalous behavior of echo signal can be observed.

Thursday, March 13, 2008 8:00AM - 11:00AM —
Session U17 DBP: Proteins in Membranes and the Cytoskeleton
Morial Convention Center 209

8:00AM U17.00001 Hierarchy of Specific Lipid-Peptide Interactions Produces the Activity of Cell-penetrating and Cell-permeating Peptides
Matthew Davis, Daniel Parente, Vernita Gordon, Abhijit Mishra, Nathan Schmidt, Lihua Yang, Robert Cordon, Abhigyan SOM, Gregory Teiw, Gerard Wong, University of Illinois, Urbana-Champaign — Protein transduction domains can cross cell membranes with high efficiency, even when carrying a variety of cargos, and thus has strong biotechnological potential. The molecular mechanism of entry, however, is not well understood. We use small-angle x-ray scattering (SAXS) and confocal microscopy to systematically study the interaction of the TAT and ANTP PTD with model membranes of variable composition. Their membrane transduction activity requires the presence of both PE and PS lipids in the membrane. Antimicrobial peptides (AMP’s) are cationic amphiphiles that comprise a key component of innate immunity. Synthetic analogs of AMP’s, such as the family of phenylene ethynylene antimicrobial oligomers (AMO’s), recently demonstrated broad-spectrum antimicrobial activity, but the underlying molecular mechanism is unknown. PE lipid greatly enhances permeating activity of AMO in these membranes, synthetic analogs of AMP’s, such as the family of phenylene ethynylene antimicrobial oligomers (AMO’s), recently demonstrated broad-spectrum antimicrobial activity, but the underlying molecular mechanism is unknown. PE lipid greatly enhances permeating activity of AMO in these membranes, and rapidly increasing use of a modality which is a known human carcinogen is a cause for concern. To assess the magnitude of the problem it is necessary to establish the shape of the dose response relationship for radiation carcinogenesis. Information on radiation carcinogenesis comes from the A-bomb survivors, from occupationally exposed individuals and from radiotherapy patients. The A-bomb survivor data indicates a linear relationship between dose and the risk of solid cancers up to a dose of about 2.5 Sv. The lowest dose at which there is a significant excess cancer risk is debatable, but it would appear to be between 40 and 100 mSv. Data from the occupation exposure of nuclear workers shows an excess cancer risk at an average dose of 19.4 mSv. At the other end of the dose scale, data on second cancers in radiotherapy patients indicates that cancer risk does not continue to rise as a linear function of dose, but tends towards a plateau of 40 to 60 Gy, delivered in a fractionated regime. These data can be used to estimate the impact of diagnostic radiology at the low dose end of the dose response relationship, and the impact of new radiotherapy modalities at the high end of the dose response relationship. In the case of diagnostic radiology about 90% of the collective population dose comes from procedures (primarily CT scans) which involve doses at which there is credible evidence of an excess cancer incidence. While the risk to the individual is small and justified in a symptomatic patient, the same is not true of some screening procedures is asymptomatic individuals, and in any case the huge number of procedures must add up to a potential public health problem. In the case of radiation oncology, modern innovations such as Intensity Modulated Radiation Oncology or Proton Therapy both result in a substantial total-body dose to the patient, which must result in an increased incidence of second cancers. The technology exists to reduce these total body doses and the problem needs to be addressed.

1Supported by The National Aeronautics and Space Administration Grant NAG-9-1519 and The Department of Energy Low Dose Program grant DE-FG02-03ER63629

8:12AM U17.00002 Simulations of the pore structures for a M2GlyR derived channel forming peptide in membrane
Ahlam N. Al-Rawi, Asma Al-Rawi, Jianhan Chen, Alvaro Herrera, John Tomich, Kansas State University, Talat S. Rahman, University of Central Florida — In an effort to develop a peptide-based compound suitable for clinical use as a channel replacement therapeutic for treating channelopathies such as cystic fibrosis, we present a reductionist model that appears to capture many of the biophysical properties of an intact ion channel using short channel-forming peptides. We have developed two anion selective channel-forming peptides with near native and altered properties from the peptides derived from the glycine receptor: NK-I-M2 GlyR-P22 WT (KKKPPPVRVGLGTTTMATTTQG) and NK-I-M2 GlyR-P22 S22W (KKKPPPVRVGLGTTTMATTTQW), respectively. Starting with the two structures determined by solution multidimensional NMR (800 MHz) in SDS, we used CHARMM and NAMD to perform molecular dynamics simulations on the monomers. Using the existing experimental data, we then built an initial 5- helix assembly by altering the tilted angle, rotational angle and pore radius. We investigated the impact of the single mutation at position 22 on the structure and dynamics of the pore formed in a membrane build in a hydrated POPC lipid bilayer. Probable structures for both assemblies are presented.
8:24AM U17.00003 Membrane-mediated mechanism of amyloid oligomer toxicity in Alzheimer’s Disease. FRANK HEINRICH, Carnegie Mellon University, YURI SOKOLOV, JAMES E. HALL, University of California, Irvine, RIMA BUDVYTYTE, GINTARAS VALIUNCIS, Institute of Biochemistry, Vilnius, MATHIAS LOESCHE, Carnegie Mellon University. There is strong evidence, that soluble amyloid β (Aβ) oligomers, involved in Alzheimer’s Disease, are the primary toxic species of Aβ, although the mechanism of cell toxicity is very much debated [1]. Neuron reflectivity and electrical impedance spectroscopy assess the structural impact of Aβ (1-42) oligomers and their effect on the electrical properties of a tethered phospholipid model membrane. Two distinct and reversible peptide – membrane interactions were revealed: At low Aβ concentrations an equal incorporation of Aβ into both lipid leaflets and a compaction of the lipid membrane takes place. Aβ locally lowers the dielectric barrier for ion transport and the activation energy for ion transport through the bilayer remains significantly above that of a water-filled transmembrane pore. At high Aβ concentrations, an additional membrane thinning is observed. [1] D. E. Eliezer, J. Gen. Physiol. 128:631 (2006).

1also at the NIST Center for Neutron Research
2also at the NIST Center for Neutron Research

8:36AM U17.00004 Molecular target of synthetic antimicrobial oligomer in bacterial membranes. LIHUA YANG, VERNITA GORDON, Department of Materials Science and Engineering, University of Massachusetts, Amherst, JOHN CRONAN, David Schwab, Robijn Bruinsma, UCLA. Antimicrobial peptides consist of a key component of innate immunity for a wide range of multicellular organisms. It has been shown that natural antimicrobial peptides and their synthetic analogs have demonstrated broad-spectrum antimicrobial activity via permeating bacterial membranes selectively. Synthetic antimicrobial peptides, on the other hand, are tunable to interact with bacterial membranes through a variety of selectivity mechanisms. We investigate interactions and self-assembly using a prototypical family of antimicrobialbased on phenylene ethynylene. Results from synchrotron small angle x-ray scattering (SAXS) results and in vitro microbidassal on genetically modified ‘knock-out’ bacteria will be presented.

3Corresponding author

8:48AM U17.00005 Interaction of Arginine-Rich Peptides with Model Cell Membranes, ABHIJIT MISHRA, NATHAN SCHMIDT, VERNITA GORDON, JIANJUN CHENG, University of Illinois at Urbana-Champaign, TIMOTHY DEMING, University of California, Los Angeles, GERARD WONG, University of Illinois at Urbana-Champaign. WONG RESEARCH GROUP TEAM. — Cell-penetrating peptides have the ability to traverse the plasma membrane of eukaryotic cells. Furthermore, these peptides can transport cargo across a range of cell membranes, implying they have many potential biotechnological applications. In this study we compare the interaction of three commonly used arginine-rich cell-penetrating peptides, TAT, Penetratin, and pVEC, with model cell membranes of variable charge density and intrinsic curvature, using synchrotron small angle x-ray scattering (SAXS). To better understand the respective roles of arginine and hydrophobic residues in membrane reorganization we also examine the interaction of arginine-leucine (R60L20) block copolyptides with model membranes, as well as the relationship between membrane composition and peptide induced changes in membrane topology.

9:00AM U17.00006 Lipid and Protein Sorting during Membrane Tube Formation, HONGYUAN JIANG, THOMAS POWERS, Division of Engineering, Box D, Brown University, Providence, RI 02912 — Motivated by recent experiments that implicate the mechanical properties of membranes in lipid sorting, we examine the interplay of lipid composition and curvature in membrane tubes. We study how the dependence of bending stiffness and surface tension on membrane lipid and protein composition affects tube formation. Drawing a tube from a vesicle leads to a rearrangement of composition in which the phase of higher flexibility segregates in the tube, the region of high mean curvature. For point forcing, the force vs. extension curve can have a sharp drop just as the tube begins to form.

9:12AM U17.00007 Equilibrium Stability of Transmembrane Proteins : A Hard-Core Gas Problem. KARIM WAHBA, DAVID SCHWAB, ROBIJN BRUINSMA, UCLA. — Hydropathy plots, a moving average of amino acid hydrophobicity over a sequence, can be used to predict potential protein structure, in particular transmembrane proteins. Traditionally transmembrane regions are identified by peaks above an empirical cutoff. We treat the transmembrane segments as a one-dimensional gas of hard rods in a correlated random energy landscape. At zero temperature, where the entropic contribution due to the loops is negligible, we calculate the density profile as a function of the chemical potential in the case of the original as well as randomly generated landscapes. The density profile exhibits plateaus indicating regions where a transmembrane segment has been established. For designed versus random sequences we explore the distribution of the sizes of these plateaus and attempt to infer characteristic features that may be interpreted in terms of the stability of the protein in its inserted state.

9:24AM U17.00008 Diffusion of Transmembrane Proteins: Beyond the Saffman-Delbrück Model, TATIANA KOURIJOBA, MARK HENLE, ALEXANDER J. LEVINE, University of California, Los Angeles — The hydrodynamic model of Saffman and Delbrück [PNAS 72 311.1975] predicts that the diffusion constant D of proteins embedded in a fluid membrane exhibits a weak logarithmic dependence on the radius σ of the protein. However, recent experiments by Gambin et al. [PNAS 103 2098 (2006)] have observed a much stronger 1/2 dependence for proteins embedded in model membranes. Local interactions between a transmembrane protein and the lipids that surround it can cause the lipids to deform by, for example, stretching or compressing their tails, or by tilting their long axis with respect to the membrane’s surface. In this talk, we show that these deformations lead to additional sources of energy dissipation which cause the protein diffusion constant D ~ σ/a, as observed by Gambin et al. Our model incorporates the lipid stretch and tilt degrees of freedom into a traditional hydrodynamic model by introducing additional scalar and vector fields, respectively.

9:36AM U17.00009 Lateral organization of a non-equilibrium membrane model with immobile randomly-distributed impurities, ANDREW P. PARADIS, SUSAN R. MCKAY, Department of Physics and Astronomy, University of Maine, Orono, Maine 04469, SAMUEL T. HESS, Department of Physics and Astronomy, Institute of Molecular Biophysics, University of Maine, Orono, Maine 04469 — Cell membranes are dynamic, far-from-equilibrium systems; transport, signaling, and other membrane functions ensure that membrane lateral organization is heterogeneous across several length scales. However, many studies and simulations consider membranes as equilibrium systems. Here, we present a model of cell membranes that includes simplified endo- and exocytosis and immobile randomly-distributed impurities. The impurities take the form of fixed protein sites within the membrane, which act as potential localization zones for micro-domain rafts. We analyze the lateral organization in terms of spatial statistics through a modified Ripley K-test. This model illuminates the role of protein in a 1:1:1 mixture of saturated lipids, unsaturated lipids, and cholesterol. Additionally, this model exhibits a realistic heterogeneity of cluster sizes and shapes, and suggests conditions under which we may observe a partitioning of cholesterol in the membrane. Such simulated observations of the direct interactions between cholesterol, lipids, and protein on the molecular scale can enhance our understanding of all biophysical processes occurring within cell membranes.
action under Osmotic Pressure successfully explains a large number of experimental observations, such as density of formin speckles and variance of actin cable density. The model predicts nucleators, the actin cable dynamics are subject to spatial and temporal fluctuations. We studied actin cable dynamics with simple analytical models and whole flow of polymerized actin toward the cell center, and cable disassembly. Formin for3p associates with actin at the cable tip where it transiently polymerizes actin...

8:36AM U18.00002 Studies of Protein Folding in Non-Funneled Free Energy Landscapes1, COREY O’HERN, GREGG LOIS, JERZY BLAWZDZIEWICZ, Department of Mechanical Engineering and Department of Physics, Yale University — A theoretical framework is developed to understand the dynamics of protein folding. The key insight is that the search for the optimal conformation of the protein is influenced by the rate at which external parameters are adjusted to induce folding. A theory based on this insight predicts that (1) proteins with non-funneled free energy landscapes can fold reliably, (2) reliable folding can occur in equilibrium or out-of-equilibrium, and (3) reliable folding only occurs when the quench rate is below a limiting value, which can be calculated from measurements of the free energy. We test these predictions against numerical simulations of heteropolymers with hydrophobic and hydrophilic interactions and a single energy scale.

8:48AM U18.00003 Exploring HP protein models using Wang-Landau sampling, THOMAS WUEST, DAVID P. LANDAU, The University of Georgia, USA — The hydrophobic-polar (HP) protein model has become a standard in assessing the efficiency of computational methods for protein structure prediction as well as for exploring the statistical physics of protein folding in general. Numerous methods have been proposed to address the challenges of finding minimal energy conformations within the rough energy landscape of this lattice heteropolymer model. However, only a few studies have been dedicated to the more revealing — but also more demanding - problem of estimating the density of states which allows access to thermodynamic properties of a system at any temperature. Here, we show that Wang-Landau sampling, in connection with a suitable move set (“pull moves”), provides a powerful route for the ground state search and the precise determination of the density of states for HP sequences (with up to 100 monomers) in both, two and three dimensions. Our procedure possesses an intrinsic simplicity and overcomes the inevitable limitations inherent in other more tailored approaches. The main advantage lies in its general applicability to a broad range of lattice protein models that go beyond the scope of the HP model.

9:00AM U18.00004 ABSTRACT WITHDRAWN —


9:24AM U18.00006 Crowding Effects on the Thermodynamics of Apoflavodoxin Folding, DIRAR AL HOMOUZ, Univ of Houston — The thermodynamics of folding in Apoflavodoxin protein are studied using coarse-grained molecular dynamics simulations as a function of volume fraction of crowding agents. The stability of the folded state is enhanced in the presence of crowding agents as can be seen from the free energy diagrams. The changes in the transition state ensemble are analyzed under different crowding conditions.

9:36AM U18.00007 Protein Folding Simulation of Mutant Go Models of the Wild-Type Trpcage Protein, APICHART LINHANANTA, JUNMIN LIU, Department of Physics, Lakehead University — For the past three decades, Go models of protein folding have played important roles in the understanding of how proteins fold from random conformations to their unique native structures. Unfortunately Go models rely on known NMR or x-ray structures to construct Go interaction potentials potentially severely limit their predictive powers. In this work, we introduce a novel method for constructing Go interaction potentials of mutant proteins based on Go interaction potentials of wild type proteins. As a template we employ the all-atom Go model of the 20-residue Trp-cage protein (A. Linhananta, J. Boer and I. MackKay, J. Chem. Phys., 2005, 122, 114901) as the wild type Go model. Trp-cage mutants are constructed by replacing a Trp-cage residue with a different residue. In particular the Pro-12 residue of the Trp-cage is substituted by Trp-12 to produce the Trp2-cage mutant, whose native structure is not yet known. Monte Carlo simulations, using CHARMM force fields, are performed to determine the ground-state structure mutant. The resulting mutant structures are used to construct the Go interaction potential of the Trp2-cage mutant model.
9:48AM U18.00008 Statistical features of the rough energy landscape of proteins emerging from single-molecule force-clamp spectroscopy. JASNA BRUJIC, MAXIME CLUSEL, ERIC CORWIN, New York University. Following the complete folding trajectories of single ubiquitin molecules opens an unique window into the detailed mechanisms of protein folding. The biological importance of this problem motivated extensive studies using macroscopic biochemistry experiments and molecular dynamics simulations at the atomic scale, while little is known about the mesoscopic mechanisms of folding. To this end, our recent experiments combined with the tools of modern statistical mechanics reveal a wealth of new information. Using this single molecule approach, we have observed physical features reminiscent of glassy systems, exemplified by a power-law distribution of the rates of protein unfolding under a stretching force [1]. To further probe the signs of complexity in protein dynamics, we investigate memory effects and the influence of force on the folding trajectories, and more specifically the mechanism of formation of native interactions. The general aim of this research is to build a self-consistent picture of the free energy landscape of proteins. [1] J. Brujic et al., Nature Physics, vol 2, 282 (2006).

10:00AM U18.00009 Asymmetrical collapse of charged heterogeneous macromolecules. NATALIJA DENESYUK, JOHN WEEKS, Institute for Physical Science and Technology, University of Maryland, College Park. We propose a new method based on local molecular field (LFM) theory to treat Coulomb interactions in simulations of ionic fluids. This method has been tested in Langevin dynamics simulations of a model protein, which consists of a random sequence of charged hydrophilic and neutral hydrophobic monomers, in salt solution. The concentration of salt ions in the simulation box is maintained by grand canonical Monte Carlo. Our general strategy is to perform averages over an ensemble of sequences in order to identify those general properties that are sequence independent. We find that, independently of their random sequence, heterogeneous polyelectrolytes undergo the asymmetrical collapse in which one of their quadrupole moments vanishes.

10:12AM U18.00101 A Model for the Thermally Induced Polymer Coil-to-Globule Transition. DAVID SIMMONS, Univ. of Texas, ISAAC SANCHEZ, Univ. of Texas. A quantitative mean-field model for the thermally-induced (heating-induced) polymer coil-to-globule transition (HCGT) is developed with no adjustable parameters. The transition temperature $\Theta$ is given for a long chain by the equation $\Theta = T_p^* \left( 1 - \tilde{\rho}(\Theta) \right)$ where $T_p^*$ is the characteristic temperature of the polymer for the lattice fluid model and $\tilde{\rho}(\Theta)$ is the reduced solvent density at the transition temperature $\Theta$. Calculated HCGT temperatures show good agreement with experimental LCSTs. The physics of the HCGT transition is shown to be consistent with the physics of the LCST transition. The predicted globular state is characterized by the dominance of attractive polymer self interactions over excluded volume interactions. This model can be easily generalized to treat cross-linked gels and their contraction-expansion characteristics.

10:24AM U18.00111 Force Induced Globule-to-Coil Transition of Single Polymer Chains. NIKHIL GUNARI, University of Pittsburgh, GILBERT WALKER, University of Toronto. Force induced structural transitions of individual homopolymer chains have been studied in different solvent conditions using single molecule force spectroscopy. Single molecule mechanics in the “fly-fishing” mode showed a first-order like transition for polystyrene (PS) in water exhibiting a characteristic three regime force extension curve. In contrast, poly methylmethacrylate (PMMA) showed a characteristic saw-tooth pattern reminiscent of multidomain disassembly behavior similar to that seen in modular protein mechanics. The plateau force for PS and the saw-tooth pattern for PMMA disappear when measured in aqueous guanidine hydrochloride solution and in other non-solvents showing that the characteristic deformational behavior observed for the two polymers in water may be due to hydrophobic interactions.

10:36AM U18.00112 Wang-Landau sampling for homopolymer collapse. DANIEL T. SEATON, STEVEN J. MITCHELL, DAVID P. LANDAU, University of Georgia. We explore the behavior of a continuum-homopolymer model using the Wang-Landau algorithm, concentrating on phase transitions such as the coil-globule and solid-liquid transitions. Using the density of states generated by the Wang-Landau algorithm, we calculate various thermodynamic quantities, e.g., the internal energy and specific heat. We also study how algorithmic parameters, such as sampling boundaries (maximum and minimum energies for random walks) and the final value of the modification factor, affect these quantities. In particular, we observe how the sampling boundaries can significantly alter the transition behavior. Our results are compared with two recent studies that yielded contradictory results, one using the bond-fluctuation model and the other using a continuum model similar to our own. We find that the transitions seen in our model are much more similar to those in the bond-fluctuation study. The careful analysis of the effects of algorithmic parameters on thermodynamic quantities should be relevant to the study of other polymeric/protein models.

10:48AM U18.00113 Stimuli-Responsive, Concentrated Aqueous Solutions of DMAEMA-containing Amphiphilic Di- and Triblock Copolymers. KYLE GUICE, Department of Chemical Engineering, University of Texas at Austin, YUEH-LIN LOO, Department of Chemical Engineering, Princeton University. Poly(dimethyoaminoethyl methacrylate), poly(DMAEMA), has generated considerable interest due to its responsiveness to changes in temperature and pH. The pendant tertiary amine groups of DMAEMA are easily protonated below its pKa, and the polymer undergoes a hydrophilic-to-hydrophobic transition when heated above its lower critical solution temperature (LCST) in water. We have investigated di- and triblock copolymers containing statistical copolymers of DMAEMA and hydroxethyl methacrylate (HEMA), a biocompatible but nonresponsive monomer, as stimuli-responsive concentrated aqueous solutions. The swelling characteristics of these concentrated aqueous block copolymer solutions depend highly on the DMAEMA composition. Further, by selecting an appropriate hydrophobic block, we are able to design stimuli-responsive concentrated aqueous solutions that undergo reversible phase transformations over a narrow temperature window.

Thursday, March 13, 2008 8:00AM - 10:48AM
Session U19 DCOMP: Computational Methods: Dynamics, Transport, and Plasma

8:00AM U19.00001 ABSTRACT WITHDRAWN

8:12AM U19.00002 Charged particle and neutron energy deposition in an inertial confinement fusion plasma leading to internal tritium breeding. KARABI GHOSH, S.V.G. MENON, Theoretical Physics Division, Bhabha Atomic Research Centre. Plasma heating by charged particles and neutrons, energy exchange between ions and electrons and radiative losses are the primary mechanisms determining the ignition conditions in a thermonuclear plasma. In this work the energy leakage probability has been obtained numerically by including the effect of nuclear scattering, small and large angle Coulomb scattering and collective plasma effects. A simple multigroup approach has been developed for energy deposition by neutrons due to nuclear interaction with the ions. Using this accurate model for energy deposition, the concept of internal tritium breeding in DT fusion pellet has been re-evaluated by numerically solving the rate equations for various participating species and energy balance equations for ions, electrons and radiation within the three temperature model. Internal tritium breeding is found to occur even when all the radiation loss mechanisms such as bremsstrahlung and inverse compton scattering are fully accounted for.
8:24AM U19.00003 Breakeven Fusion in Staged Z Pinch1, HAFIZ RAHM AN, University of California, PAUL NEY, Mount San Jacinto College, NORMAN ROSTOKER, FRANK WESSEL, University of California — We are studying the prospect for breakeven thermonuclear fusion considering a Mega joule (MJ) class, 100 ns, impulse generator using a modified version of MACH2, a 2-1/2 D, radiation-code. The load is a cylindrical, xenon plasma shell that implodes radially onto a co-axial, deuterium-tritium plasma target. Optimized plasma density and pinch radius lead to a fusion-energy output that is many times the stored capacitor bank energy. In this “Staged Z-pinch” shock fronts form that preheat the DT plasma to several hundred eV, before adiabatic compression. During compression, the Xe liner becomes Rayleigh-Taylor (RT) unstable while the DT target remains stable. Proper selection of the initial pinch radius and plasma density is crucial for optimum implosion efficiency.

1Supported by the US Department of Energy.

8:36AM U19.00004 Intensity correlations in wave transport through complex media. GABRIEL CWILICH, Department of Physics - Yeshiva University, LUIS FROUFE-PEREZ, Laboratoire EM2C, Ecole Centrale Paris, ANTONIO GARCIA-MARTIN, Instituto de Microelectronica de Madrid, CSIC, JUAN JOSE SAENZ, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid — The intensity-intensity correlations that appear when a wave propagates coherently through a random medium will be discussed within the framework of the random matrix theory (RMT) of transport. We will consider the case of transmitted-transmitted, reflected-reflected and transmitted-reflected correlations. In the case of transmission the spatial correlations can be expressed as the sums of three terms with distinctive spatial dependences. This result coincides with the one obtained in the diffusive regime from perturbative calculations, but here its validity is extended from the quasi ballistic to the localized regime. In the RMT framework, approximate solutions of the DMPK equations allow us to study the dependence of the correlations with the length of the system.

8:48AM U19.00005 Modified Transition Matrix Methods1, DAVID YEVICK, MICHAEL REIMER, BJARNE TROMBORG, University of Waterloo — Recently we adapted the transition matrix Monte-Carlo method to general communication systems problems [D. Yevick and M. Reimer, Photon. Technol. Lett. 1529 (2007), IEEE Trans. Commun., submitted, (2007)]. In this presentation, we compare the accuracy and parameter dependence of different multicanonical and transition-matrix methods. We find that the standard multicanonical method can be reformulated more simply and accurately for a single system observable (output variable) within a transition matrix formulation by constructing the intermediate probability density function (density of states) after a small number of Markov transitions from the ratios of the elements of the transition matrix between adjacent histogram bins. Further, we consider an alternative procedure in which transitions only occur either from a given state to itself or to states that have previously been less frequently sampled. Here we show that the numerical error is small unless the self-transition probability is considerable. In this case, despite the violation of detailed balance, numerical precision can be effectively restored by ensuring that the random walker thermalizes within each histogram bin before effecting a transition to a different bin.

1The National Science and Engineering Research Council of Canada (NSERC) and the Canadian Institute for Photonic Innovation (CIPI) are acknowledged for financial support.

9:00AM U19.00006 ABSTRACT WITHDRAWN —

9:12AM U19.00007 Critical phenomena of Site-Percolation Models with Two Different Sizes of Particles on a Square Lattice, RYOJI SAHARA, HIROSHI MIZUSEKI, Institute for Materials Research, Tohoku University, KIYOSHI KANIE, ATSUSHI MURAMATSU, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, YOSHIIKI KAWAZOE, Institute for Materials Research, Tohoku University, IMR, TOHOKU UNIVERSITY TEAM — The concept of percolation plays an important role in explaining various important physical phenomena, including transport, mechanical, and electromagnetic properties of disordered systems. To date, many percolation models have been developed. Contrary to the ordinary site percolation models with homogeneous particles, systems have a certain particle-size distribution. Such a distribution may affect the properties of the system in certain ways. In the present study, site-percolation models with two different sizes of particles are systematically introduced on a square lattice to understand the effect of nonhomogeneity of the particles in the system. To estimate the critical phenomena with high accuracy, a finite-size scaling analysis is performed with a Monte Carlo simulation. The critical coverage at the percolation threshold is examined as a function of the size distribution of elements in the system. Fractal dimension and the critical exponents are also estimated.

9:24AM U19.00008 Development of a Simple Sintering Law for Fractal Aggregates Composed of Unequal Sized Primary Particles1 , TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — Sintering of silicon nanoparticle chain aggregates composed of unequal sized primary particles are investigated using molecular dynamics (MD) simulations at 1500 K. We consider straight chain aggregates consisting of up to 40 2.5 and 5.4 nm primary particles. The sintering time increases with increase in the total volume of the chain aggregate or with increase in the exposed initial surface area of the chain. A mathematical model was developed to describe the dynamics of sintering of such chain aggregates. The model is a power law modification of the Frenkel sintering equation with the Koch-Friedelander model to include primary particle size dependence. We found that the particle size effect is a local process, and important only at the initial stage of the sintering. Thus, the effect is not significant when the aggregate becomes large. The model is amenable for use in aerosol models that might include sintering effects.

1NSF, AHP/CRNC

9:36AM U19.00009 Toward a new criteria of soliton/ domain wall creation in condensed matter systems?, ANDREW BECKWITH, APS/ Fermi contractor — We do an extension of prior work where we applied a quasi 1-Dimensional wavefunctional formulation of tunneling Hamiltonians to a physical transport problem characterized by a perturbed washboard potential. To do so beforehand in the quasi one dimensional situation, we considered tunneling between states that were modeled as wavefunctionals of a scalar quantum field. I-E curves that matched Zener curves — were used to fit data from an experimental standpoint with quasi one dimensional wavefunctionals congruent with the false vacuum hypothesis. We generalize this to the case of higher dimensional formulations of the wave functions, and also present a minimum criteria for the formation of soliton/ instanton structure in higher dimensions.
9:48AM U19.00010 Use of Space-Time Basis Sets for Solving Initial-Value Problems\textsuperscript{1}, CHARLES WEATHERFORD, XINGJUN ZHANG, Florida A&M University — A new algorithm for solving Quantum Mechanical initial-value problems such as the time-dependent Schrödinger equation and the Liouville equation is described. The method avoids the use of the time-translation operator which inevitably results in an essentially sequential algorithm and instead turns the problem into the solution of simultaneous equations, which produces a highly parallelizable algorithm. A basis set in time as well as spatial degrees of freedom is used. The basis may be spectral, finite element, or spectral element and may be continuous or discrete (discrete variable representation–DVR). The time-axis may have an arbitrary size of time element including only one element. The larger the time step, the larger the size of the time basis that is required. The Hamiltonian may be time-independent or time-dependent. In the case of a time-independent Hamiltonian, an extremely efficient algorithm results. For the time-dependent case, the problem of time-ordering does not arise. Several applications involving laser-atom interactions will be given.

\textsuperscript{1}Supported by the National Science Foundation and the U.S. Army

10:00AM U19.00011 Propagating the nonlinear Schrödinger equation, FREDERICK STRAUCH, Gettysburg College — We derive an exact propagation scheme for nonlinear Schrödinger equations. This scheme, analogous to the propagation of linear Schrödinger equations, results from a special operator whose properties ensure the correct propagation. Using this scheme we prove the correctness of higher-order integrators for the Gross-Pitaevskii equation and its multi-component generalizations.

10:12AM U19.00012 Reconstructing the dynamics of water sheared between charged plates using inelastic x-ray scattering, GHEE HWEE LAI, ROBERT H. CORIDAN, NATHAN W. SCHMIDT, PETER M. ABBAMONTE, GERARD C. L. WONG, UIUC — Understanding the dynamical behavior of water under confinement or near surfaces is fundamental to tribology and many transport processes in cell biology. To achieve angstrom and femtosecond resolution in water dynamics, we reconstruct the space-time longitudinal (density) response function from high-resolution inelastic x-ray scattering (IXS) studies of water and, together with linear response theory, investigate how water behaves between two moving 2-D charge lattices at different charge densities and inter-plate separations. We find that the density profile varies with plate separation with a periodicity close to the diameter of a water molecule (~2.6Å), in agreement with surface forces apparatus measurements, and that the hydration patterns of charges on the surfaces are strongly velocity dependent.

10:24AM U19.00013 Ergodicity of Isothermal Molecular Dynamics Method\textsuperscript{1}, HIROSHI WATANABE, Nagoya University — A condition for equations of motion for isothermal dynamics is derived, and the Nosé–Hoover method is generalized on the basis of this condition. The ergodicity of the one-variable thermostats are studied, and it is shown that the one-variable thermostat coupled with the one-dimensional harmonic oscillator loses its ergodicity with large enough relaxation time. A stochastic process of the Nosé–Hoover method is also discussed based on the Markovian approximation.

\textsuperscript{1}This research was partially supported by the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Young Scientists (B), 19740235, 2007.

10:36AM U19.00014 Statistical Mechanics of the Fluctuating Lattice Boltzmann Equation, BURKHARD DUENWEG, ULF SCHILLER, Max Planck Institute for Polymer Research, Mainz, Germany, ANTHONY J.C. LADD, Chemical Engineering, University of Florida, Gainesville, USA — The statistics of the occupation variables of a stochastic lattice Boltzmann simulation is analyzed in terms of a generalized lattice gas. We show that the most probable state of this model corresponds to the equilibrium distribution of the lattice Boltzmann equation. Stochastic collision rules are described in terms of a Monte Carlo process satisfying detailed balance. This allows a straightforward derivation of the discrete Langevin equation for the fluctuating modes. Detailed balance requires to thermalize all non-conserved modes. A Chapman–Enskog analysis shows that the approach is fully consistent with macroscopic fluctuating hydrodynamics.

Thursday, March 13, 2008 8:00AM - 11:00AM – Session U20 DMP: Focus Session: Metal Surfaces, Interfaces, and Thin Films Morial Convention Center 212

8:00AM U20.00001 Surface islands nucleated by a beam of energetic self-ions on Pt(111): A low-energy electron microscopy study\textsuperscript{1}, MICHAL ONDREJCEK, C. PETER FLYNN, WACEK SWIECH, University of Illinois at Urbana-Champaign — Using low energy electron microscopy (LEEM), we observe the adatom and advacancy islands nucleate and evolve when clean Pt(111), in the temperature range 750-1300K, is bombarded by a beam of Pt\textsuperscript{+} ions of various energies. The source of negative ion beam is incident on the sample at normal incidence with impact energies selectable in the range of 0 to 5 keV, and with current densities up to 40 µA/cm\textsuperscript{2}. We describe briefly initial experiments done with LEEM-ion accelerator tandem namely the investigations of relaxing steps extending the range over which surface mass diffusion coefficient D\textsubscript{a} is

\textsuperscript{1}This research was supported by U.S. Department of Energy through grants DEFG02-02ER46011 and DEFG02-91-ER45439.

8:12AM U20.00002 The effect of Fe atoms on the adsorption of a W atom on W surfaces, JEFFERY HOUZE, SUNGKYO KIM, SEONG-JIN PARK, RANDALL GERMAN, MARK HORSTEMEYER, SEONG-GON KIM, Mississippi State University — We report ab-initio calculations on the effect of iron (Fe) atoms on the adsorption of a tungsten (W) atom on W(100), W(110), and W(111) surfaces. The adsorption of a W atom on the clean W surfaces is compared with the adsorption of a W atom on a monolayer of Fe atoms covering the W surfaces. The total energy of the system is computed as the function of the height of the W adatom. For the W(100) surface I will show that the W atom first adsorbs onto the Fe monolayer. Then the W atom can replace one of the Fe atoms through a path with a moderate energy barrier and reduce its energy further. This intermediate site makes the adsorption (and desorption) of W atoms a two-step process in the presence of Fe atoms and lowers the overall adsorption energy by nearly 2.4 eV. Similar processes for adsorption will be presented for the (110) and (111) surfaces. Our result provides a fundamental mechanism that can explain the activated sintering of tungsten by Fe atoms.
8:24AM U20.00003 Stability of V and Ti on Al surfaces: Searching for suitable interlayer materials to stabilize the Fe-Al interface. WEERASINGHE PRIYANTHA, HUI CHEN, MICHAEL KOPCZYK, KASEY LUND, DAN TOWN, RICHARD SMITH, Montana State University, Bozeman, MT. PONNUSAMY NACHIMUTHU, VAITHYALINGAM SHUTTHANANDAN, Pacific Northwest National Laboratory, Richland, WA — There is considerable interest in fabricating thin film multilayer structures with sharp interfaces for a wide variety of applications. Interface intermixing may degrade the desired physical properties of a structure, but this may be reduced in some cases using stabilizing interlayers at the interface. Model calculations predict that both V and Ti will be effective stabilizing interlayers for the Fe-Al interface, a system well known for considerable intermixing at room temperature. We have used X-ray reflectometry (XRR) and Rutherford backscattering spectrometry (RBS) to characterize bilayers and trilayers of the Fe-V-Al and Fe-Ti-Al systems prepared using dc magnetron sputtering. Our analysis revealed that Fe-Al bilayer systems showed considerable intermixing, especially when the Fe layer was deposited on top of the Al. It was also found that with V or Ti as an interlayer at the interface, the intermixing of Fe and Al was reduced.

8:36AM U20.00004 Magic planar Ag clusters. Y.P. CHIU, C.M. WEI, C.S. CHANG, TIEN. T. TSONG, DEPARTMENT OF PHYSICS, NATIONAL SUN YAT-SEN UNIVERSITY, KAOSHIUNG, TAIWAN, ROC COLLABORATION, INSTITUTE OF PHYSICS, ACADEMIA SINICA, TAIPEI, TAIWAN, ROC COLLABORATION, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA, TAIPEI, TAIWAN, ROC COLLABORATION — The spontaneous assembly of atoms and molecules in a system has attracted many research interests and created numerous potential applications. Utilizing the periodic pattern found on the Pb quantum islands, which are grown on the Si(111) surface, we have recently discovered that self-organized Ag planar clusters formed on these templates exhibit enhanced stability at some particular sizes. Detailed calculations based on ab initio density functional theory have also been performed. The use of a density-functional optimization in geometrical structures and the corresponding binding energy support an examination of the genesis of these magic Ag nanoclusters and their relative stability. When the Ag nanopuck grows to a certain size, the geometrical effect takes hold from the electronic effect as the major attribute, which drive the Ag nanopucks towards well defined hexagonal crystalline structures. The theoretically related electronic and geometrical structures are also correlated with the experimentally energetically favorable structures of these magic clusters.

8:48AM U20.00005 Crucial electronic contributions to measures of surface diffusion by He atom scattering. GUIDO FRATESI, ETSF and Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, IT. GIL ALEXANDROWICZ, Cavendish Laboratory, University of Cambridge, Cambridge, UK, MARIO ITALO TRIONI, ETSF and CNISM, UdR Milano-Bicocca, Milano, IT, GIAN PAOLO BRIVIO, ETSF, CNISM, and Dipartimento di Scienze dei Materiali, Università di Milano-Bicocca, Milano, IT, WILLIAM ALLISON, Cavendish Laboratory, University of Cambridge, Cambridge, UK — In a He atom scattering (HAS) experiment, the position and motion of atoms or molecules at a surface is inferred indirectly, through the electron distribution at the sample surface. Nevertheless, surface diffusion measurements are typically analyzed assuming that the electron distribution simply follows the position of the surface atoms. We have examined theoretically recent HAS measurements of Na/Cu(001), identifying a non trivial relation between the dynamics of the electron distribution and that of the Na ions. The magnitude of the calculated variations in the charge density, and their dependence on the atomic density of adsorbates, account for the correlated 3D motion experimentally observed. The results of this study further highlight the sensitivity of HAS to the electron distribution of the sample and point out the role of electronic contributions in high-resolution measures of surface dynamics.

9:00AM U20.00006 Sapphire Surface Polymorphs and The Growth of Pb Overlayers. HAWOONG HONG, Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana-Champaign, AARON GRAY, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana-Champaign, T.-C. CHIANG, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana-Champaign — The surface structure of sapphire (α-alumina) is an issue of long-standing interest, both scientifically and technologically. Molecular dynamics simulations showed the γ-alumina structure to have a lower energy than that of α-alumina [1], thus suggesting a possibly modified surface structure when sapphire is treated at high temperatures. We have performed x-ray reflectivity measurements at the Advanced Photon Source to address this issue. Standard sapphire substrates were prepared by furnace annealing at 1600° C in air. The resulting surfaces showed large terraces with straight step edges. The substrates were then annealed in a UHV chamber at increasingly higher temperatures. Many new features emerged in the reflectivity curves, which could be attributed to various transition alumina structures, including the δ-, θ-, and θ' polymorphs [2]. Pb films were grown on these surfaces. The resulting structure and morphology was characterized. This talk will summarize our findings. [1] S. Blonski and S. H. Garofalini, Surf. Sci. 295, 263 (1993). [2] I. Levin and D. Brandon, J. Am. Ceram. Soc. 81, 1995 (1998).

9:12AM U20.00007 Molecular dynamics simulations of low temperature Cu/Cu(100) growth. VALERY BOROVIKOV, YUNISC SHIM, JACQUES G. AMAR, University of Toledo — Recent X-ray scattering studies [1] of Cu/Cu(100) growth indicate the existence of a sharp transition from epitaxial growth at high temperatures to growth with a high vacuum concentration at lower temperatures (T < 150 K). Here we present the results of molecular dynamics (MD) simulations carried out in order to understand the detailed mechanisms of incorporation of vacancies and voids (vacancy clusters) into the growing film during low temperature deposition. The dependence of compressive strain, vacancy concentration and vacancy-cluster size distribution in deposited thin film, as well as the surface roughness and morphology on deposition conditions, such as the growth temperature, deposition angle, and incident kinetic energy will be discussed and compared with experiments. [1] C. E. Botez, K. Li, E. D. Lu, W. C. Elliott, P. F. Miceli, E. H. Conrad, and P.W. Stephens, Appl. Phys. Lett. 81, 4718 (2002).

9:24AM U20.00008 Parallel temperature accelerated dynamics simulations of vacancy formation in low temperature Cu/Cu(100) growth. YUNISC SHIM, VALERY BOROVIKOV, JACQUES G. AMAR, University of Toledo, BLAS P. UBERUAGA, ARTHUR F. VOTER, Los Alamos National Laboratory — While molecular dynamics simulations may be used to study thin-film growth at very low temperatures and at very high deposition rates, in order to study growth over time scales close to experiment, accelerated dynamics simulations are needed. Here we present the results of parallel temperature-accelerated dynamics simulations of low-temperature Cu/Cu(100) growth carried out using our recently developed parallel temperature-accelerated dynamics (parTAD) method, in order to understand recent X-ray diffraction experiments showing a surprisingly large vacancy concentration in Cu(100) growth at low temperature. In general, we find that, due to the existence of increased surface relaxation and activated events, the vacancy concentration obtained in our parTAD simulations is smaller than the corresponding concentration obtained in molecular dynamics (MD) simulations. The dependence of compressive strain and vacancy concentration, as well as the surface roughness and morphology, on growth temperature and deposition angle will also be discussed and compared with experiments.
9:36AM U20.00009 Atomic Processes responsible for the diffusion of 2D Cu islands on Ag(111): results from self learning KMC. O. TRUSHIN, Institute of Microelectronics, ASR, Yaroslavl, H. YILDIRIM, A. KARA, T.S. RAHMAN, Department of Physics, University of Central Florida — Diffusion on Ag(111) of small 2D-Cu clusters (4 to 30 atoms) is examined using embedded atom method potentials, as a first step towards understanding hetero epitaxial growth. A combination of an Off-Lattice Self-Learning Kinetic Monte Carlo and spherical repulsion scheme for saddle point searches, has revealed novel diffusion mechanisms. For this size range, the diffusion of islands involves 3 classes of processes: i) collective concerted motion (gliding), found to be dominant for small sized islands (4-9); ii) processes involving shear mechanism in which some of the Cu island atoms are commensurate with the substrate and others are not (≥ 9 atoms), finally iii) processes involving a “breathing” mechanism in which the island “shrinks” as a whole before “relaxing” to a less compact shape with a net displacement of the whole cluster equivalent to an fcc-hcp hop (≥ 12 atoms). These processes were revealed during the first 100 KMC steps for each island. Diffusion coefficients as a function of temperatures, effective diffusion barriers and frequencies of the responsible events will be presented.

1This work was supported in part by NSF-ITR 0428826.

9:48AM U20.00010 Semi-coherent Fe(001)/MX(001) interfaces, DAN FORS, GÖRAN WAHNSTRÖM, Chalmers University of Technology — Using ab initio calculations we investigate interface energies and structures for the semi-coherent Fe(001)/MX(001) interface systems. We apply a continuum approach using the Peierls-Nabarro model in order to account for the elastic displacements arising from the lattice mismatch and the periodic misfit dislocations in the interface. The chemical part of the interface energy is obtained by using density functional theory calculations. We find that the Fe/MN systems show decreasing trends along the 3d, 4d and 5d element rows corresponding to stronger bonding to Fe. In contrast the Fe/MC systems show a maximum for the Ti group. The trends and differences have been explored using projected density of states and charge density analysis. The results show a strong covalent bonding between Fe and C(N) when the two atoms are aligned on top of each other, but the hybridization itself can’t account for the differences along the rows. Instead the trend appears to be due to the metallic interaction between the Fe atom and M atom in the interface layer. We also find that the Fe/MX-interfaces have large misfits, which causes that many atoms will be unfavorable positioned and the elastic energy will constitute a significant part of the interface energy.

10:00AM U20.00011 Unstable and metastable states of dynamics governed by surface diffusion, B. DAVIDOVITCH, H. KING, C.D. SANTANGELO, UMass — Under certain kinetic conditions, the dynamics of solid surfaces is governed by surface diffusion processes. This type of dynamics is relevant, for example, in high-temperature sintering processes, and in the coarsening of nanorods metals coated by catalytic elements. For compact surfaces, the fixed points of this dynamics are surfaces of constant mean curvature (CMC). It is thus natural to ask whether there exist nontrivial CMC’s which are stable under dynamics governed by surface diffusion. This question will be addressed in this talk. We will discuss some subtleties concerning an analytic approach to the problem, and will present some numerical results for simple CMC surfaces.

10:12AM U20.00012 Morphology evolution of solid thin films in the presence of long range de-wetting interactions, ADI CONSTANTINESCU, West Virginia University, ARTEM LEVANDOVSKY, University of California Riverside, LEONARDO GOLUBOVIC, West Virginia University — The thin films of metals, such as cobalt or silver on substrates such as sapphire exhibit a striking formation of multilayered islands that reach heights many times larger than the initial film thickness. Here, we theoretically elucidate these phenomena within an interface dynamics model which incorporates both Mullins type surface diffusion relaxation and long range de-wetting forces acting across the film, such as Van der Waals forces and Ferminomial Casimir forces (Quantum size effect). The model is used to explore the scaling laws of multilayered island height growth as well as the coarsening laws governing surface evolution. At early times, the surface evolution is dominated by strong up-hill surface currents caused by long range Casimir-like forces. At late times however, the surface coarsening laws are universal and dominated by surface tension effects.

10:24AM U20.00013 Charge Transfer Model for Dissociative Barrier Formation; A First Principles Study, SHIGEYUKI TAKAGI, HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University — The origin of the formation of the barriers has been explained, for two decades, using Pauli repulsion, i.e., exchange term, by Hammer et al.[1] Excluding the exchange term in the electronic total energy calculation, we have however obtained the monotonic increase of the potential energy surface in the dissociation process of the H₂ molecule on Au(111) system. So we propose another origin for the formation focusing on the charger transfer induced by electronegativity differences between the hydrogen molecule and Au metal surfaces using density functional calculations. We evaluate the charges that belong to atoms in the system during the dissociation process using Bader analysis. The calculated dissociation energy curve along the reaction path coincides with that of the isolated, separated and positively charged hydrogen molecule using the linear combination of the atomic orbital method in real space. No interaction between the hydrogen molecule and the Au surface has been found in the initial stage of the dissociation. The transfer elongates the inter-atomic distance of the hydrogen molecule that raises the energy of the molecule, leading to the formation of the energy barrier in the present case. This charge transfer model is confirmed to be applicable to not only the present system but also H₂/Mg, H₂/Pt, O₂/Pt systems. [1] B. Hammer and J.K. Nørskov, Nature 376, 238 (1995).

10:36AM U20.00014 A Density Functional Study of Atomic Hydrogen and Oxygen Chemisorptions on the (0001) Surface of Double Hexagonal Close Packed Americium, PRATIK DHOLABHAI, RAYMOND ATTA-FYNN, ASOK RAY, The University of Texas at Arlington — Ab initio total energy calculations within the framework of density functional theory have been performed for atomic hydrogen and oxygen chemisorptions on the (0001) surface of double hexagonal packed americium using a full-potential all-electron linearized augmented plane wave plus local orbitals (FLAPW+lo) method. The three-fold hollow hcp site was found to be the most stable site for O adsorption. Chemisorption energies and adsorption geometries for different adsorption sites will be discussed. The change in work functions, magnetic moments, partial charges inside muffin-tins, difference charge density distributions and density of states for the bare Am slab and the Am slab after adsorption of the adatom will be discussed. The implications of chemisorption on Am 5f electron localization-delocalization will also be discussed.

3This work is supported by the U. S. Department of Energy and the Welch Foundation, Houston, Texas.

10:48AM U20.00015 Simulations of adsorption of hydrocarbons on decagonal AlNiCo quasicrystal surfaces, WAHYU SETYAWAN, Duke University, RENEE D. DIEHL, MILTON W. COLE, Pennsylvania State University, STEFANO CURTAROLO, Duke University — Classical many-body interatomic potentials for hydrocarbon adsorptions on Al-Ni-Co systems are developed by using the Embedded-Atom Method. The potentials are fit to ab-initio energies of Al-Ni-Co ternary phases and hydrocarbons adsorbed on decagonal surface of Al-Ni-Co (d-AlNiCo) approximants. First principle data show that no dissociation occurs for all systems in the training set, indicating no chemisorptions. We extend the study and use the potentials to simulate adsorption of simple hydrocarbons on d-Al2Ni3Co13 quasicrystal surfaces using Grand Canonical Monte Carlo method. Research sponsored by ACS and NSF.
Fourier analysis was conducted and no significant frequencies could be distinguished.

calculate the contact angles was developed, resulting in values of 2.7 ± 0.14 Pa. A

environment. In at least two of the cylinders, the liquid-vapour interface adopted a two-interface configuration, as previously predicted. An initial analysis was

based on this analysis was inferred to be 3.3 ± 0.14 Pa. A

chloroform colloidal suspensions. We examine anchoring as a function of interface shape and droplet size and discuss the impact on liquid

were considered monodisperse. Finally, we consider in the patterned substrate case cells with a prescribed number of colloids and characterize these deposits.

1 Work supported by NSF grant DMR-0305194

2 Supported by NSF grant number DMR-0240078.

8:36AM U21.00004 Binary mixture study of CF\textsubscript{4} and CF\textsubscript{3}Cl on graphite\textsuperscript{1}, PETROS THOMAS, DANIEL VELAZQUEZ, GEORGE HESS, University of Virginia — In a binary mixture adsorption study of CF\textsubscript{4} and CF\textsubscript{3}Cl on graphite from 60 K to 105 K, both the CF\textsubscript{3}Cl - ν\textsubscript{as} and the CF\textsubscript{4} - ν\textsubscript{as} frequency shifts are measured using IRAS as the spreading pressure (chemical potential) of CF\textsubscript{4} is increased. Even though CF\textsubscript{4} has a much lower saturation vapor pressure (SVP) compared to CF\textsubscript{3}Cl (at 80 K, SVP of CF\textsubscript{4} is ∼ 70 mT and that of CF\textsubscript{3}Cl is ∼ 0.1 mT), the CF\textsubscript{4} either continuously dissociates or adsorbs on top of CF\textsubscript{3}Cl depending on the initial coverage of CF\textsubscript{3}Cl on the graphite surface. For temperatures between 70 K and 105 K we also lower coverage of CF\textsubscript{3}Cl, where the molecules lie with their C – Cl axis nearly parallel with the surface, the CF\textsubscript{3}Cl continuously displaces CF\textsubscript{4} from the surface. For saturated monolayer coverage of CF\textsubscript{4}Cl, where the C – Cl axis of the molecules is tilted relative to the surface, the CF\textsubscript{4}Cl molecules adsorb on top of the CF\textsubscript{3}Cl – HOPG template. At 60 K, the displacement of the low-coverage CF\textsubscript{3}Cl is only partial and the orientation of the remaining CF\textsubscript{4}Cl is tilted relative to the surface from a nearly flat position.

1 Work supported by NSF grant DMR-0305194

8:48AM U21.00005 DFT Estimation of Lateral Interactions in Lattice-gas Models of Br and Cl on Ag(100)\textsuperscript{1}, T. JUWONO, P.A. RIKVOLD, Florida State University — We studied Br and Cl chemisorbed on a Ag(100) surface, using a lattice-gas model and the Density Functional Theory (DFT) method. In this model the Br and Cl ions adsorb at the fourfold hollow sites of the Ag(100) surface, which yields a square lattice of adsorption sites. Five different coverages for each kind of adsorbate were calculated. For each adsorbate and coverage, we obtained the minimum-energy configuration, its energy, and its charge distribution. From these data we calculated dipole moments, lateral interaction energies, and binding energies. Our results showed that for Br the lattice-gas model obtained by fitting to the adsorption energies from the DFT calculation is consistent with long-range dipole-dipole lateral interactions using the dipole moments calculated from DFT charge distribution. For Cl we found less consistency, which indicates that long-range dipole-dipole interactions are not sufficient to describe the Chlorine system.

1Supported by NSF grant number DMR-0240078.
9:24AM U21.00008 Dissipation at Moving Contact Lines: Effect of Interface Width and Slip

MARK ROBBINS, SHENGFENG CHENG, Johns Hopkins University, COLIN DENNISTON, University of Western Ontario — Continuum mechanics predicts a diverging stress and total dissipation when the contact line between a fluid interface and a solid substrate is advanced. Several models for removing this divergence have been advanced. One is that the divergence is cutoff by a finite slip length. Another is that diffusion can remove the singularity for fluid interfaces of finite width. Extensive molecular dynamics simulations of partially miscible binary fluids were used to test these two pictures. The interfacial tension was changed by a factor of 20 and the interfacial width by an order of magnitude. The interface width had no direct effect on the dissipation and diffusion was orthogonal to the predicted direction. The dissipation only depended on system size, the dimensionless capillary number, and the slip length $S$ associated with the flow boundary condition in the fluid far from the contact line. The divergence in stress is cut off at the sum of $S$ and a distance of order the molecular diameter. The dissipation rises rapidly as the amount of slip is decreased. In all cases there is a first order transition where the advancing contact line becomes unstable and a film is entrained.

9:36AM U21.00009 Counterintuitive connection between layering and mobility in confined fluids

GAURAV GOEL, WILLIAM KREKELBERG, University of Texas at Austin, JEFFREY ERRINGTON, State University of New York at Buffalo, THOMAS TRUSKETT, University of Texas at Austin — Fluids confined to narrow spaces adopt a spatially inhomogeneous distribution of density due to the interactions between the fluid particles and the boundaries. This “density profile” is the most common measure of inhomogeneous structure in confined fluids, but its connection to fluid transport coefficients is poorly understood. We explore via molecular simulations how tuning particle-wall interactions to flatten or enhance the particle layering of a model Weeks-Chandler-Andersen (WCA) confined fluid impacts its self-diffusivity, viscosity, and entropy. Counterintuitively, interactions that eliminate particle layering significantly reduce confined fluid mobility, while those that enhance layering have the opposite effect. Excess entropy helps to both understand and predict these trends.

9:48AM U21.00010 Effective interfacial tension between miscible fluids

JOHN POJMAN, The University of Southern Mississippi, NICK BESSONOVI, Institute of Problems of Mechanical Engineering, GLORIA VINER, The University of Southern Mississippi, VITALY VOLPERT, Université Lyon I — Isobutyric acid (IBA) and water have an Upper Critical Solution Temperature of 27 Celsius. Using spinning drop tensiometry, we were able to demonstrate the existence of an effective interfacial tension by preparing a drop of isobutyric acid-rich phase below the UCST and then raising the temperature above the UCST. The capillary instability was also observed by rapidly reducing the rotation rate. We also demonstrated that such an effective interfacial tension is not unique to the IBA-water systems but can also occur in the cyclohexane – aniline, which has a Lower Critical Solution Temperature.
Driving proteins and DNA with mechanical forces: Pushing, pulling, and squeezing molecules using computer simulations.\textsuperscript{1} \textsuperscript{1}NSF, Welch Foundation

Fluorescent resonant energy transfer: Correlated fluctuations of donor and acceptor\textsuperscript{2}. ZHI-GANG YU, SRI International — Mounting evidence suggests that in single-molecule fluorescent resonant energy transfer (FRET) measurements, correlation between fluctuations in donor and acceptor may be important. We present a general theory to describe this correlation and its effect on the FRET rate\textsuperscript{1}. The correlation arises from low-energy excitations (e.g. acoustic phonons) of the molecule to which a donor-acceptor pair is attached, and results in an effective interaction between local environments or baths associated with the donor and the acceptor. The correlation is found to reduce the transfer rate, in particular at short donor-acceptor distances. The theory can quantitatively explain recent measurements of polyproline peptides.\textsuperscript{1} Z. G. Yu, J. Chem. Phys. 27, 20xxxx (Communications) (2007).

The water effects on long-distance charge transfer in polypeptides. NIKOLAISERGUEEV, ALEXANDERDEMKOV, The University of Texas at Austin — Long-range electron transfer (ET) is one of the most intriguing reactions occurring in biological systems. Recent experiments indicate that water play an important role in the mechanism of charge transfer in proteins. In this talk we present the first-principles study of the effect of intervening water molecules on the electron tunneling processes in simple polypeptide bridges. The ET rate is related to the probability current flow which is computed using density functional theory and nonequilibrium Green’s function formalism which takes into account the inelastic electron-phonon scattering in the bridge. Our results suggest that the effect of water is two fold. First, the insertion of water molecules changes the conformational probability current that is computed using density functional theory and nonequilibrium Green’s function formalism which takes into account the inelastic electron-phonon scattering in the bridge. Our results suggest that the effect of water is two fold. First, the insertion of water molecules changes the conformational

In\textsubscript{2}O\textsubscript{3} nanowire based field effect transistor for biological sensors. ZHONGMINGZENG, KAIWANG, WEILIEZHOU, Advanced Materials Research Institute, University of New Orleans, New Orleans, LA 70148 — Semiconductor nanowires (NWs) are attracting considerable attention due to their nanoscale dimensions and enormous surface-to-volume ratios. Many applications have been demonstrated in toxic gas, protein, small molecule and viruses sensing because of their superior sensing performances. Indium oxide (In\textsubscript{2}O\textsubscript{3}) NWs are working as n-type channel with obvious back-gate effect, which is much stronger than the reported results. The nanodevices used as virus detection will be also discussed.

Messenger RNA sequence and the translation process—a particle transport perspective\textsuperscript{1}. JIAJIA DONG, BEATE SCHMITTMANN, ROYCEK.P. ZIA, Virginia Tech — The translation process in bacteria has been under intensive study. A key question concerns the quantitative effect of different elongation rates, associated with different codons, on the overall translation efficiency. Starting with a simple particle transport model, the totally asymmetric simple exclusion process (TASEP), we incorporate the essential components of the translation process: Ribosomes, cognate tRNA concentrations, and messenger RNA (mRNA) templates correspond to particles, hopping rates, and the underlying lattice, respectively. Using simulations and mean-field approximations to obtain the stationary currents (the protein production rates) associated with different mRNA sequences, we are especially interested in the effect of slow codons, i.e., codons which are associated with rare tRNAs and are therefore translated very slowly. As a first step, we look at a “designed sequence” with one and two slow codons and quantify the marked impact of their spatial distribution to the currents. Extending the results to several mRNA sequences taken from real genes, we argue that an effective translation rate including the information from the vicinity of each codon needs to be taken into consideration when seeking an efficient strategy to optimize the protein production.

Sticky-sphere model for phase separation of mixtures of the eye lens proteins gamma-B and alpha crystallin: non-monotonic dependence on mutual attraction. GEORGETHURSTON, MAURINOBAUTISTA, DAVIDROSS, VERNLINDBERG, HOSSEINSHAHMOHAMAD, Rochester Institute of Technology — We apply a multi-component extension of the Baxter sticky-sphere model to aqueous solutions of the eye lens proteins gamma-B crystallin and alpha crystallin. These mixtures show liquid-liquid phase separation induced by gamma-B/gamma-B attraction, gamma-B/alpha size disparity and gamma-B/alpha attraction. We examine the dependence of the upper-critical spinodal temperature surface on gamma-B/alpha attraction, previously found to influence stability. Gamma-B crystallin is modeled with a temperature-dependent stickiness parameter that reproduces both static light scattering and small-angle neutron scattering near its critical point. Alpha crystallin is modeled as a hard sphere. We find that the Barbo-Teene model shows a non-monotonic dependence of the spinodal temperature surface on gamma-B/alpha attraction that is qualitatively consistent with recent molecular dynamics simulation results. Hard-sphere or very attractive gamma-B/alpha interactions lead to instability, and the spinodal surface shows a minimum in an intermediate range of gamma-B/alpha attraction strength. We examine the nature of the two types of instability.
9:36AM U22.00007 Structural Isotopic Effects in the smallest chiral amino acid: Observation of a structural phase transition in fully deuterated alanine. HELIOISA BORDALLO1, HMI, JOELMA DE SOUZA, PAULO DE TARSO, Universidade Federal do Ceará, DIMITRI ARGYRIOU, HMI — A first study of possible changes instigated by deuteration in amino acids was carried out using neutron diffraction, inelastic neutron scattering and Raman scattering in L-alanine, C\textsubscript{2}H\textsubscript{4}(NH\textsubscript{2})COOH. Careful analysis of the structural parameters shows that deuteration of L-alanine engenders significant geometric changes as a function of temperature, which can be directly related to the observation of new lattice vibration modes in the Raman spectra. The combination of the experimental results suggests that C\textsubscript{2}D\textsubscript{4}(ND\textsubscript{2})COOD undergoes a structural phase transition (or a structural rearrangement) at about 170 K. Considering that this particular amino acid is a hydrogen-bonded system with short hydrogen bonds (O...H \sim 1.8 Å), we evoke the Ubbelohde effect to conclude that substitution of hydrogen for deuterium gives rise to changes in the hydrogen-bonding interactions. The structural differences suggest distinct relative stabilities for the hydrogenous and deuterated L-alanine. De Souza et al. - Journal of Physical Chemistry B (Letters) 111, 5034-39 (2007)

1 bordallo@hmi.de

9:48AM U22.00008 Exploring the Electrical Conductivity of Myoglobin\textsuperscript{1}. DEBIN LI, DAVID LEDERMAN, Dept of Physics, West Virginia University, PETER M. GANNETT, Basic Pharmaceutical Sciences, West Virginia University — The electrical conductance of single myoglobin proteins was measured to study its electron transfer properties. We examined the electronic properties of myoglobin, using apomyoglobin (myoglobin without a heme group) as a reference. The differential conductivity of the proteins deposited on Pt nanometer-scale electrodes was measured using a lock-in technique as a function of bias and gate voltages. Nano- electrodes were fabricated by creating small Pt channels 100 nm - 300 nm wide via e-beam lithography and then creating a break junction by electromigration at low temperatures (4 K - 77 K). The conductance of apomyoglobin was very different from that of myoglobin, with a predominant peak at 50 meV. On the other hand, myoglobin had a rich structure that we surmise results from the presence of the heme group.

\textsuperscript{1}Supported by the WVNano Initiative at West Virginia University

10:00AM U22.00009 Selective binding affinity of cationic antimicrobial peptides for lipid membranes: roles of peptide charge and hydrophobicity\textsuperscript{1}. SATTAR TAHERI-ARAGHI, BAE-YEUN HA, Department of Physics and Astronomy, University of Waterloo, Ontario N2L 3G1, Canada — Antimicrobial peptides selectively disrupt microbial membranes through hydrophobic insertion into the outer layers, which are known to carry a large fraction of anionic lipids. When the peptides are cationic, as is often the case, the interplay between hydrophobic and electrostatic interactions determines the selective binding affinity (thus antimicrobial activity) of the peptides. Here we present a detailed theoretical picture of how the selective binding is influenced by such factors as the charge and hydrophobicity of the peptides and the elasticity of target membranes. This effort not only accounts for some of the general trends observed in experimental studies, but it also leads to a theoretical model for optimizing the selectivity and antimicrobial activity.

\textsuperscript{1}This work was supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada

10:12AM U22.00010 Excitation dynamics in purple bacteria photosynthetic membranes under different light adaptation conditions . FELIPE CAYCEDO, FERNEY RODRIGUEZ, LUIS QUIROGA, Universidad de los Andes — Photosynthetic membranes in \textit{R. Sphaeroides} purple bacteria adapt to light growth conditions such as the intensity level of radiation, which determine their amount of Reaction Centers (RCs), and also their global architecture. In any case, for both high and low intensity conditions the trend for core (LH1) and outer (LH2) complexes clustering is maintained. Using a Förster hopping model for excitation transfer, we analyze different adapted membranes for which we report results for the yield and lifetime of excitations under continuous illumination levels. We show that complexes stoichiometry obey to efficiency optimization amount of Reaction Centers (RCs), and also their global architecture. In any case, for both high and low intensity conditions the trend for core (LH1) and outer (LH2) complexes clustering is maintained. Using a Förster hopping model for excitation transfer, we analyze different adapted membranes for which we report results for the yield and lifetime of excitations under continuous illumination levels. We show that complexes stoichiometry obey to efficiency optimization

10:24AM U22.00011 Microscopic Electrohydrodynamics of DNA electrophoresis\textsuperscript{1}. ALEKSEI AKSENTIEV, BINQUAN LUAN, Department of Physics, University of Illinois at Urbana-Champaign — Gel electrophoresis is currently the most successful yet costly method to sequence DNA. Electrophoresis of DNA through solid-state nanopores holds promise for reducing the costs and making personal genomics a reality. The underlying physics of DNA electrophoresis, however, remains controversial. Theoretical models of this process often invoke the notion of the effective charge of a DNA molecule \(q_{\text{eff}}\) to account for the reduced electric force on DNA in an external field \(E\), i.e. \(F = q_{\text{eff}}E\). However, experimental estimates of \(q_{\text{eff}}\) can differ from each other by as much as ten times. To clarify the physical origin of the reduction of an electric force on DNA in electrophoresis, we investigated this process through extensive all-atom molecular dynamics simulations. Our results demonstrate that the effective screening of the DNA charge arises from the hydrodynamic drag of the electroosmotic flow, not from the counterion condensation. We show that the effective driving force \(F\) of an applied electric field \(E\) in a nanopore obeys the same law as in a bulk electrolyte: \(F = \xi \mu E\). Here, \(\xi\) and \(\mu\) are, respectively, the friction coefficient and electrophoretic mobility of DNA that depend on the surface properties of a nanopore, such as its roughness. Based on the above law, a method for determining the effective driving force is suggested that does not require a direct force measurement.

\textsuperscript{1}This work is supported by grants from NIH ( R01-HG003713, PHS 5 P41 RR05969) and NSF LURP MCA655028.

10:36AM U22.00012 Multivalent counterions inhibit DNA ejection from viral capsid . TOAN NGUYEN — Viral DNA packaged inside a bacteriophage is tightly bent. This stored bending energy of DNA is believed to be the main driving force to eject viral DNA into host cell upon capsid binding. One can control the amount of ejected DNA by subjecting the virus to a solution of PEG8000 molecules. The molecules cannot penetrate the viral capsid, therefore, they exert an osmotic pressure on the virus preventing DNA ejection. Experiments showed that for a given osmotic pressure, the degree of ejection also depends on the concentration of small ions in solution. Interestingly, for multivalent ions (such as Mg\textsuperscript{2+}, Spd3+ or HexCo3+), this dependence is non-monotonic. We propose a simple electrostatic theory to explain this non-monotonic behavior. This is based on the fact that DNA molecules can invert their net charge at high enough multivalent counterion concentration. In other words, as multivalent counterion concentration is increased from zero, charge of DNA molecules change from negative to positive. At the concentration where DNA net charge is zero, the DNA molecules experience an attraction between different segments and DNA ejected amount is reduced. At low or high counterion concentration, DNA segments are charged (negatively or positively), repel each other and DNA ejected amount is increased. Fitting the result of the theory to experimental data, we obtain a numerical value for Mg\textsuperscript{2+} mediated DNA - DNA attraction energy to be \(-0.008\text{kJ} \text{per base}\).

Thursday, March 13, 2008 8:00AM - 10:48AM – Session U23 DMP GMAG: Focus Session: Manganite Thin Films Morial Convention Center 215
8:00AM U23.00001 Thickness dependence of the exchange bias in epitaxial manganite bilayers*, ALEXEY KOBRINSKII. University of Minnesota, MARIA VARELA, Oak Ridge National Laboratory, ALLEN GOLDMAN, University of Minnesota, U OF MN OXIDE MBE TEAM, OAK RIDGE NATL LAB COLLABORATION — A series of thin ferromagnetic/antiferromagnetic (F/AF) bilayers of doped lanthanum manganites La$_2$/3Ca$_1$/3MnO$_3$ (F) and La$_1$/3Ca$_2$/3MnO$_3$ (AF) have been grown by ozone-assisted molecular beam epitaxy (OAMBE). The lattice of the substrate material (001) SrTiO$_3$ is a good match to that of the manganites. Growth by the OAMBE method results in samples with sharp interfaces, which are suitable systems to study the interfacial phenomenon of exchange bias (EB). We present present EB as a function of the AF layer thickness and determined two critical values of the thickness for the onset and for the saturation of the hysteresis loop shift which is traditionally used to measure the effect. The observed dependence of EB on the AF layer thickness can be described within the original or generalized Meiklejohn-Bean model. Using this simple approach we have estimated the interfacial coupling energy and the antiferromagnetic anisotropy constant.

*This work was supported by the NSF through the University of Minnesota MRSEC under Grant NSF/DMR-0212032.

8:12AM U23.00002 Infrared studies of Phase Separated (La$_{1-x}$Pr$_x$)$_{0.67}$Ca$_{0.33}$MnO$_3$ Thin Films*, NAVEEN MARGANKUNTE, TARA DHAKAL, AMLAN BISWAS, D.B. TANNER, Dept of Physics, University of Florida — We report optical spectroscopy studies of phase separated (La$_{1-x}$Pr$_x$)$_{0.67}$Ca$_{0.33}$MnO$_3$ thin films grown on the substrate NdGaO$_3$. Reflectance measurements in the far and mid infrared were performed for a range of temperatures from 10 to 300 K. Particular attention was given to the narrow temperature range where the insulator-metal transition occurs. The optical constants were extracted by fitting the measured reflectance to a Drude-Lorentz dielectric function in conjunction with thin film optics and the measured properties of the substrate. Spectral weight analyzes show that the growth of low energy oscillator strength occurs well above the Curie temperature, indicating phase coexistence in the hysteresis regime seen in resistivity measurements. The optical conductivity results are contrasted with existing models for free carrier electrodynamics in manganites.

8:24AM U23.00003 Anisotropic Magnetoresistance in (La,Pr)$_{0.67}$Ca$_{0.33}$MnO$_3$ Films, MEGUMI YAMAMOTO, CHUHEE KWON, California State University Long Beach, ANTHONY DAVIDSON, SANJAY ADHIKARI, RAJESWARI KOLAGANI, Towson University — The out-of-plane anisotropic magnetoresistance (AMR) was measured in mixed phase manganite (La,Pr)$_{0.67}$Ca$_{0.33}$MnO$_3$ (LPCMO) films. Two samples with different film thicknesses (~30 nm and ~150 nm) on LaAlO$_3$ substrate were compared for the effects of stress on AMR. The thicker sample exhibits an insulator-metal resistive transition with a hysteresis typical of LPCMO with the peak temperature of 175 K and 250 K at H = 0 T and 8 T, respectively. While the resistance of the thinner sample is too high for our system to measure (Quantum Design PPMS) below 140 K at H = 0 T, the peak temperature at 8 T is 105 K. AMR shows a sinusoidal angular dependence typical of a ferromagnet for both samples. In this talk, we will present systematic AMR measurements of the LPCMO samples. We found that the peak position of AMR depends both on film thickness and on temperature. In addition, we observed time-dependent changes in resistance at lower temperatures indicating a long relaxation time for spins.

8:36AM U23.00004 Interface magnetism in complex oxide heterostructures*, HARIRAN SRIKANTH, University of South Florida — Magnetic oxides are an important class of materials from the perspectives of fundamental physics and technological applications. Advances in growth of high quality thin films and epitaxial oxide heterostructures over the years, have led to the realization of ideal condensed matter systems in which the complex and rich physics associated with cooperative phenomena can be explored. Examples of coupled phenomena in heterostructures include exchange bias effects, magneto-electric coupling and interplay between magnetism and superconductivity. In this talk, I will focus on three classes of oxide heterostructures – PLD-grown M-type barium hexaferrite (BaM)/barium strontium titanate (BST), CVD-grown CrO$_2$/CrO$_3$ bilayers and high-pressure sputtered LCMO/YBCO films. The common theme is the magnetic coupling across the interfaces. I will demonstrate that dynamic susceptibility and kinetic inductance experiments using a sensitive tunnel-diode oscillator (TDO) are effective probes of such coupled effects. In the case of CrO$_2$/CrO$_3$ and LCMO/YBCO, the interface coupling results in anomalous anisotropy, exchange bias in the former and complex interaction between the LCMO magnetism and YBCO vortex lattice in the latter. In BaM/BST heterostructures, I will discuss how interfacial coupling influences the microwave response that is both electrically and magnetically tunable.

*Supported jointly by NSF grant DMR-0305043 and DOE contract DE-AI02-03ER46070.

9:12AM U23.00005 Atomic resolution STM study of Perovskite Manganite Thin Films, KENNJI FUCHIGAMI, University of Tennessee, ORNL and IHI Co. Ltd., Japan, ZHENG GAI, ORNL, ZHENGMING YIN, ORNL, E. WARD PLUMMER, University of Tennessee and ORNL, LIFENG YIN, ORNL, E. WARD PLUMMER, University of Tennessee and ORNL, JIAN SHEN, ORNL and University of Tennessee — The perovskite manganites have attracted huge interest due to their intriguing electronic inhomogeneous nature which is believed to be responsible for colossal magnetoresistance. Scanning tunneling microscope (STM) is one of the most promising techniques for studying such electronic inhomogeneity in real space. In order to investigate electronic property at the surface of non-layered perovskite manganite, we have synthesized single crystal La$_{5/8}$Ca$_{3/8}$MnO$_3$ (LCMO) thin film by laser MBE technique. In-situ thin film growth enables us to obtain atomically resolved STM image which has c-2x2 superlattice unit cell. In this talk, we will discuss the electronic properties as well as lattice structures of the LCMO surfaces. This research is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the US Department of Energy under Contract No. DEAC05-00OR22725.

9:24AM U23.00006 Linear Crack Arrays and Resistive Anisotropy in Nd$_{0.2}$Sr$_{0.8}$MnO$_3$ Thin Films Under Tensile Strain*, KRISHNA NEUPANE, JOSHUA COHN. University of Miami, JOHN NEUMEIER, Montana State University — The structure, morphology, and electrical properties of epitaxial c-axis oriented thin films of Nd$_{0.2}$Sr$_{0.8}$MnO$_3$ are reported for thicknesses 10 < t < 150 nm. Films with t ≥ 20 nm grown under tensile stress on NdGaO$_3$ (100) and LSAT (110) substrates develop uniform linear crack arrays (cracks running along film c axis) with a crack spacing (0.3-10 μm) that decreases with increasing thickness. Films grown under compression on LaAlO$_3$(110) substrates exhibit no cracks. The room-temperature in-plane electrical resistance ratio, ρc/ρa, increases approximately exponentially with increasing film thickness to values of ~1000 in the thickest films studied. The temperature dependencies for ρc and ρa are approximately identical, suggesting that very long effective transport paths perpendicular to the cracks are responsible for enhanced values of ρc.

* This material is based upon work supported by the National Science Foundation under grants DMR-0072276 (Univ. Miami) and DMR-0504769 (Montana State Univ.), the Research Corporation (Univ. Miami), and the U.S. DOE Office of Basic Energy Sciences (Grant No. DE-FG-06ER46269).
9:36AM U23.00007 Effect of strain and disorder in manganite thin films, SUNG HEE YUN, RAJIV MISRA, BEN DEGLEE, JACOB TOSADO, TARA DHAKAL, ARTHUR HEBARD, AMLAN BISWAS. Department of Physics, University of Florida — We have studied the effect of strain and disorder on the phase separated state in thin films of the manganite (La_{1-x}Pr_{x}0.67Ca_{0.33}MnO_3 (LPCMO), y = 0.4, 0.5, 0.6) grown on (110) NdGaO_3 substrates using pulsed laser deposition. Due to the competition between the charge-ordered insulating and ferromagnetic metallic phases, thin films of LPCMO display a fluid-like phase separation (FPS) near the insulator-to-metal transition temperature. By applying direct mechanical stress on the LPCMO thin films using a three-point beam bending technique, we observed a colossal piezoresistance in the FPS state of these materials. Our observations show that a small amount of strain (~10^{-3}) can move the phase boundaries in the FPS state. We then modified the extrinsic disorder in the thin films by bombarding them with Ar-ions. Our measurements show a reduction of piezoresistance in the ion-bombarded samples which suggests that such extrinsic disorder can pin the phase boundaries and reduce the fluidity of the FPS state.

9:48AM U23.00008 Low Temperature Magneto-transport Measurements on Multilayered Manganese Films1, J. M. SPENCER, P. BHUPATHI, S. H. YUN, A. BISWAS, Y. LEE. Department of Physics, University of Florida, Gainesville, FL 32611-8440 — We have performed out-of-plane resistance measurements on a micro-fabricated multilayered manganite thin film structure down to 50 mK. The structure is composed of a 26 nm thick (La_{0.67}Pr_{0.33}Ca_{0.33}MnO_3 (LPCMO) film on top of a 60 nm thick (La_{0.67}Ca_{0.33}MnO_3) (LCMO) layer grown on an (110) NdGaO_3 (NGO) substrate. Two gold electrodes were deposited on the LPCMO layer and the exposed LCMO layer was then etched by ion plasma etching technique. We observed an upturn in resistance below 30 K for various current excitations ranging from 0.2 to 100 µA. Based on the electric and magnetic field dependence of the resistance, we attribute the upturn to the disorder-induced static phase separation of the LPCMO thin film at low temperature.

1This work is supported by NSF grant no. DMR-0299483 (Y.L.)

10:00AM U23.00009 The influence of growth temperature on the physical properties of La1-xSrxMnO3 thin film by rf magnetron sputtering, YONHANG PEI, JIWEI LU, STUART WOLF — Perovskite La_{1-x}Sr_{x}MnO_{3} has been of interest for such diverse applications as a spin injector for spintronic devices and for fuel cell electrodes due to its magnetic and transport properties, namely high spin polarization and ionic conduction. In this work, we prepared La_{1-x}Sr_{x}MnO_{3} thin films by rf-magnetron sputtering. LSMO films were deposited on single crystal SrTiO_{3} (100) substrates and platinized Si wafers concurrently in the temperature range from 450 to 600 °C. X-Ray diffraction (XRD) determined that the LSMO film was epitaxial on either substrate. Magnetic hysteresis loops were measured at temperatures between 10 and 300K and the saturation moment was significantly improved by increasing the growth temperature. In addition, the Curie temperature of LSMO was between 150 and 250 K and was also strongly dependent on the growth temperature. We will also discuss the impact of growth temperature on the temperature dependent transport and magnetic properties of LSMO.

10:12AM U23.00010 Current-induced and Photoinduced Effects in Annealed Bi1−xCa0.5MnO3 Thin Films1, VERA SMOLYANINOVA, K. KARKI, RAJESWARI KOLAGANI, G. YONG, R. KENNEDY. Towson University — Doped rare-earth manganese oxides exhibit a wide variety of physical phenomena. Application of magnetic field, electric field, or electromagnetic wave irradiation drastically modifies electrical conductivity and refraction index of these materials. A photoinduced and current-induced insulator to metal transition in charge-ordered (CO) manganese oxides is especially interesting from the point of view of photonic and opto-electronic device development. We have found that 50 nm Bi_{0.4}Ca_{0.6}MnO_{3} thin film grown on NdCaAlO_{4} substrate is very susceptible to increase of current and illumination with laser light (λ ~ 500 nm) [1]. Application of these stimuli partially destroys CO and produces charge-disordered conductive phase. Combined application of illumination and current completely destroys the charge ordering in this material, while the application of one of these factors separately is not sufficient to produce such effect. Current-induced and photoinduced properties of the Bi_{0.4}Ca_{0.6}MnO_{3} thin films grown on different substrates will also be presented and current-voltage characteristics will be discussed. [1] V. N. Smolyaninova at al., Phys. Rev. B 76, 104423 (2007).

1This work is supported by the NSF grants DMR-0348939 and DMR-0453342.

10:24AM U23.00011 Enhancement of Photoinduced Effects in Annealed Bi1−xCa0.5MnO3 Thin Films, K. KARKI, RAJESWARI KOLAGANI, G. YONG, R. KENNEDY, K. DEMARCHI, VERA SMOLYANINOVA, Towson University — Doped rare-earth manganese oxides (manganites) exhibit a rich variety of interesting physical phenomena including their sensitivity to application of magnetic, electric fields, and electromagnetic wave irradiation. A photoinduced insulator to conductor transition in charge-ordered (CO) manganites is especially interesting from the point of view of creating photonic devices. Thin films of Bi_{0.4}Ca_{0.6}MnO_{3} exhibit large photoinduced effects associated with melting of the charge ordering by visible light and can support conducting and insulating phase coexistence on a submicron scale [1]. We have found significant increase of the photoinduced resistivity changes and the life time of the photoinduced conducting phase after annealing. The changes in current-induced effects in annealed films will be also reported, and the possible origin of these effects will be discussed. [1] V. N. Smolyaninova at al., Phys. Rev. B 76, 104423 (2007).

1This work is supported by the NSF grants DMR-0348939 and DMR-0453342.

10:36AM U23.00012 Insulating Domain Walls in Mixed Phase Manganite, GUNEETA SINGH BHALLA, S. SELCUK, T. DHAKAL, A. BISWAS, A.F. HEBARD. — We present here evidence of novel insulating domain walls (IDWs) which allow direct tunneling of spin polarized currents in thin films of the mixed phase ferromagnet (La_{0.4}Pr_{0.6}Ca_{0.3}MnO_{3}). Elastic interactions in the distorted perovskite structure of (La_{0.4}Pr_{0.6}Ca_{0.3})MnO_{3} coupled with magnetostatic interactions give rise to coexisting ferromagnetic metallic and insulating regions near the Curie temperature, T_{C}. Well below T_{C}, magnetization measurements reveal that the mixed phase metal/insulator state evolves into a fully saturated ferromagnetic metallic state. However, when either the film thickness is reduced, or a thicker film is patterned into a nanometer wide bridge structure, the formation of domain structure is modified as theoretically predicted for mixed phase ferromagnets, resulting in thin IDWs separating adjacent half-metallic domains. Experimentally we observe that upon cooling below T_{C}, a predominantly ferromagnetic supercooled state persists where remnants of the insulating regions behave as IDWs within the bridge. Tunneling across IDWs results in metastable, temperature-independent, high-resistance plateaus over a large range of temperatures below T_{C}. Upon application of fields on the order of the coercive field, neighboring domains align and the IDWs are extinguished resulting in sharp, collosal resistance drops. The presence of IDWs offers rich physical insights into ferromagnetic domain formation in mixed phase systems.

Thursday, March 13, 2008 8:00AM - 10:48AM — Session U24:DMP: Focus Session: Transport in Nanostructures VI: Nonequilibrium Phenomena and Noise. Morial Convention Center 216
8:00AM U24.00001 Imaging hot-electron transport using chemical reactions on metal surfaces

PETRO MAKSYMOWICH, Oak Ridge National Laboratory — We have investigated a new regime of single-molecule excitation in the scanning tunneling microscope, where hot electrons locally injected from the STM tip spread out via surface resonances over length scales of up to 100 nm and electronically excite surrounding molecules causing chemical reactions. Such non-local reactions were observed for several different molecules on the (111), (110) and (100) terminated surfaces of gold and copper. The hot-electron origin of these reactions was differentiated from the possible electric field effect in the tip-surface junction on the basis of the statistical analysis of the dissociation yield as well as the non-local excitation in the presence of artificially fabricated nanoclusters. One of the new opportunities provided by the non-local excitation is a direct measurement of hot-electron transport on a metal surface. Using a phenomenological kinetic model for the statistical analysis of the non-local reactions, it is shown that the reaction rate increases linearly with tunneling current and decays exponentially with the distance from the excitation pulse. Since the attenuation length of the non-local reaction has little dependence on the STM-tip and the parameters of the excitation, we argue that it is proportional to the inelastic mean-free path of hot-electrons in the surface resonance. The angular distribution of the reaction events is isotropic on Au(111), which is consistent with the symmetry of its surface resonances in the energy range of the non-local reaction. It is also shown that the total yield of the non-local reaction provides a measure of hot-electron transport across single-atom steps. Although the reflectance of the hot-electrons by single atom steps on Au(111) is less than 20% at energies above 1.5 V, the yield of the reaction becomes surprisingly asymmetric if hot-electrons are injected in the immediate vicinity of the step.

8:36AM U24.00002 Electromigration force, surface resistivity and low-frequency noise

ALEXANDER ABANOV, Stony Brook University, DMITRI IVANOV, Ecole Polytechnique Fédérale de Lausanne — We derive constraints on the statistics of the charge transfer between two conductors in the model of arbitrary time-dependent instant scattering of non-interacting fermions. ALEXANDER ABANOV, Stony Brook University, DMITRI IVANOV, Ecole Polytechnique Fédérale de Lausanne — Scattering of charge carriers from surface structures will become an increasing factor in the resistivity as the structure decreases in size to the nanoscale. The measured effects of scattering at the most basic surface defect, a kink in a step edge, are 5x larger than for a freely diffusing surface atom. For thermally active materials, this yields a corresponding contribution of the fluctuating steps to the surface resistivity, which will exceed 1% of the bulk resistivity as wire diameters decrease below 10s of nanometers. The temporal fluctuations of kink density will cause resistivity noise. Relating the known fluctuation spectrum of the step displacements to fluctuations in their lengths, the corresponding resistivity noise is predicted to show spectral signatures of $\sim f^{-1/2}$ for step fluctuations governed by random attachment/detachment, and $\sim f^{-3/4}$ for step fluctuations governed by step-edge diffusion.

1 Supported by NSF-MRSEC at UMD.

8:48AM U24.00003 ABSTRACT WITHDRAWN

9:00AM U24.00004 Frequency-dependent counting statistics in interacting nanoscale conductors

RAMON AGUADO, DAVID MARCOS, CSIC, CLIVE EMARY, TOBIAS BRANDES, TU Berlin — Following the considerable success of shot-noise in the understanding of transport through mesoscopic systems, attention is now turning towards the higher-order statistics of electron current. The so-called Full Counting Statistics (FCS) of electron transport yields all moments (or cumulants) of the probability distribution $P(n,t)$ of the number of transferred electrons during time $t$. The theory of FCS is now well established in the zero-frequency limit. However, this is by no means the full picture, since the higher-order current correlators at finite frequencies contain much more information than their zero-frequency counterparts. In this work [1], we present a formalism to calculate finite-frequency current correlations in interacting nanoscopic conductors. We work within the n-resolved density matrix approach and obtain a multi-time cumulant generating function that provides the fluctuation statistics solely from the spectral decomposition of the Liouvillian. We apply the method to the frequency-dependent third cumulant of the current through a single resonant level and through a double quantum dot. Our results, which show that deviations from Poissonian behaviour strongly depend on frequency, demonstrate the importance of finite-frequency higher-order cumulants in fully characterizing transport.


9:12AM U24.00005 ABSTRACT WITHDRAWN

9:24AM U24.00006 Nonequilibrium elastic quantum transport using plane waves

ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC), Donostia, Spain, LIN-WANG WANG, Lawrence Berkeley National Laboratory (LBNL), Berkeley, USA — In this work, we present an ab initio nonequilibrium electronic structure method for modeling the elastic electron transport through a nanostructure coupled to semi-infinite external electrodes and with an applied bias voltage. Our method is based on the scheme presented in Ref. [1], where the coherent quantum transport is calculated by means of the exact scattering states of the system obtained using plane waves and for zero applied bias voltage. In the case of a finite bias voltage, the electronic system is in a nonequilibrium situation, and the problem needs to be solved self-consistently. Here, we present an approach to obtain the self-consistent charge density and potential of the system, which are then employed in the calculation of the nonequilibrium transmission coefficient and conductance. As an illustration, results for a model system made up of a di-thiol-benzene (DBT) molecule connected by two Cu wires are provided. [1] A. García-Lekue and L.W. Wang, Phys. Rev. B, 74, 245404 (2006).

3 This work was supported by U.S. Department of Energy, BES, under contract No.DE-AC02-05CH11231 and used the resource of the National Energy Research Scientific Computing Center.

9:36AM U24.00007 Allowed charge transfers between coherent conductors driven by a time-dependent scatterer

ALEXANDER ABANOV, Stony Brook University, DMITRI IVANOV, Ecole Polytechnique Fédérale de Lausanne — We derive constraints on the statistics of the charge transfer between two conductors in the model of arbitrary time-dependent instant scattering of non-interacting fermions at zero temperature. The constraints are formulated in terms of analytic properties of the generating function: its zeroes must lie on the negative real axis. This result generalizes existing studies for scattering by a time-independent scatterer under time-dependent bias voltage. We discuss the meaning and possible extensions of our results.

9:48AM U24.00008 Ab-initio formulation of the 4-point conductance of interacting electronic systems and its implementation in the GWST method

PETER BOKES, Dept. of Physics, University of York, York, U.K. and Dept. of Physics, Slovak University of Technology, Bratislava, Slovakia, MATTHIEU VERSTRAETE, Dept. of Physics, University of York, York, U.K., REX GODBY, Dept. of Physics, University of York, U.K. — The commonly employed linear-response expression for the conductance of quantum junctions suffers from an ambiguity of the definition of the applied potential difference. We show how this is resolved in terms of the formally as well as physically well defined 4-point conductance [P. Bokes, J. Jung, and R. W. Godby, Phys. Rev. B 76, 125433 (2007)]. Furthermore, expressing the 4 point conductance solely in terms of the density response function or polarizability, we obtain a computationally viable approach to go beyond mean-field, Green’s function based descriptions of realistic ab initio models of quantum junctions. We will discuss the numerical implementation of the formalism within the GWST code for the real-space imaginary-time GW method [N. Rojas, R.W. Godby and R.J. Needs, Phys. Rev. Lett. 74 1827 (1995)] and present results for several simple systems.

4 This work was supported by the NATO Security Through Science Programme (EAP.RIG.981521) and the EU’s 6th FP through the NANOQUANTA Network of Excellence (NMP4-CT-2004-500198).
Comparison of transport calculations using complex absorbing potentials and the Non-equilibrium Green's function formalism. Kalman Varga, Joseph Driscoll, Vanderbilt University, Nashville — In the Non-equilibrium Green's formalism (NEGF) the system is divided into left and right leads and a central region. To avoid spurious reflections from the boundaries one has to treat the leads as semi-infinite systems. Various efficient recursion methods are developed [1] for this purpose. Alternatively, one can use a complex absorbing potential (CAP) that absorbs the outgoing waves and one only has to deal with short finite leads. In this work we have compared the NEGF recursion and CAP approaches (1) on a simple analytically solvable example and (2) by calculating the transmission coefficients for a carbon nanotube device using a density functional Hamiltonian. Both approaches give very accurate results but the CAP method is orders of magnitude faster in calculating the self-energies. This work was supported by NSF grant ECS 0622146.

Systematic Study on Quantum Confinement and Waveguide Effects for Elastic and Inelastic Currents in Atomic Gold Wire: Importance of the Phase Factor for Modeling Electrodes, Hisao Nakamura, Koichi Yamashita, Univ. of Tokyo — Quantum confinement of the electrodes is an important issue for electron transport through molecular or atomic wire junctions. To assess the importance of waveguide effects by quantum confinement of the electrodes, we have calculated elastic and inelastic conductance and inelastic electron tunneling spectra of atomic gold wire with gold electrodes for several models. The results show the quite important role of the phase factors between the modeled electrodes and the contact region.

Nonlinear transport properties of model metal–Mott-insulator–metal heterostructures, Satoshi Okamoto, Materials Science and Technology Division, Oak Ridge National Laboratory — Transport properties of heterostructures in which a finite number of correlated-insulator or correlated-metal layers are sandwiched by semi-infinite metallic leads are investigated by using the layer dynamical-mean-field method combined with the Keldysh Green’s function technique. We use as impurity solvers the equation-of-motion decoupling method, the noncrossing approximation and the iteration perturbation method. Electron spectral functions in the interacting region are shown to evolve by an applied bias voltage. These effects control the current-voltage characteristics of the heterostructures. It is also shown that the deformed spectral functions strongly affect the optical response. These features differentiate a correlation-induced Mott insulator and a conventional band insulator.

1 This work was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy.

Phonon Effects on Charge Transport Through a Two State Molecule, Sergio E. Ulloa, Efta Yudiarsha, Ohio University — We study the effect of local and non-local phonon on the transport properties of a molecule model described by two electronic states. The local phonon interaction is tackled by means of a Lang-Firsov transformation [1,2]. The interaction with non-local phonons (phonon-assisted hopping) is considered perturbatively up to the first nonzero order in the self energy. The presence of different kinds of electron-phonon interaction open new transmission channels. In addition to the polaron shift and replicas due to local phonons, non-local phonons cause the appearance of new satellite states around the initial states. In the weak coupling regime of non-local phonon and electrons, states are shifted an amount proportional to square of the interaction. However, in the strong coupling regime, the non-linear effects emerge and display more interesting features on transport properties. Additional features on transport properties due to new transmission channel are shown to appear at finite temperatures. [1] G. D. Mahan, Many-particle physics, 3rd ed. (Plenum Publishers, New York, 2000). [2] R. Gutierrez et al., Phys. Rev. B. 74, 235105 (2006).

1 Supported by OU-BNNT.

Thursday, March 13, 2008 8:00AM - 11:00AM –
Session U25 DPOLY: Theory and Simulation II Morial Convention Center 217

Monte Carlo simulations of a coarse-grain model for block-copolymer melts: method and application, Francois Detcheverry, Darin Pike, Paul Nealey, Juan De Pablo, Department of Chemical and Biological Engineering, University of Wisconsin - Madison, Madison, WI 53706, Marcus Mueller, Institut fur Theoretische Physik, Georg-August Universitat, 37077 Goettingen, Germany — A new Monte Carlo based approach has been developed for simulation of polymeric systems, including block copolymers. The approach represents the system at the level of a coarse-grain Hamiltonian, akin to that employed in widely used self-consistent field theoretic (SCFT) treatments. In contrast to traditional implementations of SCFT, however, molecules are treated explicitly and fluctuations are taken into account. We present two distinct implementations of the method; the first relies on a grid and the second does not. While the grid-based method is highly computationally efficient, the gridless implementation permits simulations in arbitrary ensembles, including the grand-canonical and Gibbs ensembles, thereby facilitating study of phase transitions. The gridless implementation also gives access to the local mechanical properties. The performance of the two implementations is discussed in the context of several applications, including the directed assembly of multi-block copolymer thin films on patterned substrates, either chemical or topographical. In both cases we examine the ordering of the material and the effect of pattern or surface roughness.

Interaction between Polymer Grafted Particles: Self-Consistent-Field Study, Jaeup Kim, Mark Matsen, University of Reading — Recently, there has been an ongoing debate regarding a possible attraction between two polymer grafted nanoparticles. Using numerical self-consistent field theory (SCFT) we investigate the inter-particle potential, showing that only a monotonically increasing repulsive force is expected between the two particles regardless of the particle size and brush thickness. We also compared the exact mean-field result to approximate solutions using the Derjaguin approximation. The previously reported attraction is thought to be an anomaly caused by the use of bispHERical coordinates. We avoid this problem by developing a new SCFT scheme using two separate spherical coordinate systems centered on each particle. The idea of using multiple coordinate systems is applicable for many polymeric problems involving complicated geometries. In this scheme, two or more coordinate systems share an overlapping volume. Then the statistics of the polymers belonging to a certain coordinate system are solved in trial fields, and the resulting polymer concentration is shared by all coordinate systems to find a self-consistent solution. This method has been tried for other problems such as the behavior of a Janus nanoparticle (solved in spherical coordinates) in block copolymer lamellar phase (solved in cylindrical coordinates).

1 This work was supported by EPSRC (EP/D031494).
constant $T = 0.8$ by changing the LJ well depth ($\epsilon$).

This observation is confirmed by calculating the density profile of each cylinder and Fourier transform of the density distribution. We also performed jumps at

8:36AM U25.00004 Cylindrical phase of diblock copolymers in thin films. MARIANNE BREUER, BARBARA DROSSEL, Technical University of Darmstadt — We investigate the microphases of diblock copolymers confined in a thin film with walls attracting one of the monomer types. We focus on the possible structures of copolymers that form cylindrical phases in the bulk. We employ both self-consistent field theory and strong segregation theory to obtain the concentration profile minimizing the free energy of the system and to compare the free energy of possible morphologies. We present a phase diagram showing the possible microphases for a diblock copolymer with fixed volume fraction and fixed segregation parameter in dependence of the film thickness and the affinity of the walls. We study the effects of numerical inaccuracies on the appearance of different morphologies and their free energies.

8:48AM U25.00005 Cubic Micellar Crystals of $A_nB_mA_n$ Block Copolymers from MD. CHRIS LORENZEN, Kings College London, JOSHUA ANDERSON, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Amphiphilic block copolymers exhibit a wide variety of phases in solution. One common phase of $A_nB_mA_n$ polymers is made up of spherical micelles with hydrophobic (B) cores and hydrophilic (A) coronas. At high enough concentrations, these micelles order on a lattice forming a micellar crystal. The dynamics during the formation of this phase are fascinating, being controlled almost entirely by the polymer transfer between micelles, as shown in Molecular Dynamics simulations. Application of a standard nucleation and growth analysis shows that the micellar crystals grow extremely rapidly and are probably aided by the periodic box in the simulation. A study of the dynamics at equilibrium shows that polymer transfer is still a continuing process and can be understood in the context of transition state theory.

3Supported through DOE contract no. DE-AC02-07CH11358 and NSF grant DMR-0426597

9:00AM U25.00006 Brownian Dynamics Simulation of Kinetics of HEX Cylinders to FCC Spheres Transition in ABA Triblock Copolymer in Selective Solvent. MINGHAI LI, Boston University, RAMA BANSIL2, Boston University and National Science Foundation — We report Brownian Dynamics simulations on 400 bead-spring chains of triblock copolymer, $A_1B_2A_1$, in a selective solvent for the A block using a FENE potential together with Lennard-Jones (LJ) for B-B attraction and a Weeks-Chandler-Anderson potential for A-B and A-A repulsions. On varying volume fraction and temperature $T$ (in units of $\epsilon/k_B$, where $\epsilon$ is the well depth of the LJ interaction and $k_B$ the Boltzmann constant) we observe spheres in cubic phases, HEX cylinders, worm-like and disordered micelles. The time evolution following a quench from $T=0.0$ to a temperature $T>0.0$ shows a nucleation and growth mechanism where one cylinder breaks into spheres and induces neighboring cylinders to break into spheres. This observation is confirmed by calculating the density profile of each cylinder and Fourier transform of the density distribution. We also performed jumps at constant $T=0.8$ by changing the LJ well depth ($\epsilon$) from 1 to various higher values. We found that for $\epsilon > 4$ the cylinders are kinetically trapped, and the transition is fastest for $\epsilon = 1.5$.

1Supported by NSF DMR and IR/D support from NSF to RB.

2On Leave at NSF

9:12AM U25.00007 Thermal and Mechanical Properties of Polymer Nanofibers from Molecular Simulations. SEZEN CURGUL, KRYSYNY J. VAN VLJET, GREGORY C. RUTLEDGE, MIT — Polymer nanofibers exhibit new, emergent behavior as the diameter of the fibers are decreased from macroscopic to nanometer length scales. Since individual nanofibers are challenging to characterize experimentally due to their small size, computer simulations can be helpful in predicting the properties. We present the results of molecular dynamics (MD) simulations of polymer nanofibers to study their size-dependent properties. The fibers mimic the prototypical polymer polyethylene and have diameters in the range 2.0 to 23.0 nm. The fibers have been analyzed size dependent behavior in their thermal and mechanical properties. The glass transition temperature ($T_g$) of these amorphous nanofibers decreases with decreasing fiber diameter, and is independent of molecular weight over the range considered. Application of a volume averaged layer model for $T_g$ shows that the cooperativity length scale compares well with previous estimates for polyethylene. Young’s moduli of these nanofibers also decrease with decreasing fiber diameter, in agreement with $T_g$ depression. There is a significant decrease in modulus when the temperature increases above the glass transition temperature of the surface layer.

9:24AM U25.00008 ABSTRACT WITHDRAWN —

9:36AM U25.00009 Predicting glass transition temperatures from simulation studies. SOLOMON DUKI, PHILIP TAYLOR, Case Western Reserve University — We have been seeking techniques by means of which the glass transition temperature $T_g$ of a polymer can be predicted with minimal computational effort. With this goal in mind, the glass transition in syndiotactic poly(methyl methacrylate) was studied through atomistic molecular-dynamics simulations performed at temperatures in the range from 320 K to 700 K. The mean squared deviations of atoms, monomers, and molecules from their initial positions were analyzed by several different techniques. The most direct method looks at the long-time diffusive motion, and detects a characteristic change in the diffusion constant at $T_g$. This approach required lengthy computer runs to achieve meaningful results. Other techniques study the velocity correlation functions and the short-time translational motion. All three yield identical values for $T_g$, but it is found that the method that is most economical of computing resources is the analysis of the short-time departure from ballistic behavior. The apparent softening of the “cage” in which a monomer or chain segment oscillates coincides with the onset of diffusive motion.

1Work supported by DOE Grant DE-FG02-05ER46244

9:48AM U25.00010 Band Structure Controlled by Chiral Imprinting. ADRIAN REYES CERVANTES, Universidad Nacional Autonoma de Mexico, P. CASTRO-GARAY, RUBEN RAMOS-GARCIA, Instituto Nacional de Astronomía Óptica y Electrónica — Using the configuration of an imprinted cholesteric elastomer immersed in a racemic solvent, we find the solution of the boundary-value problem for the reflection and transmission of incident optical waves due to the elastomer. We show a significant width reduction of the reflection band for certain values of nematic penetration depth, which depends on the volume fraction of molecules from the solvent, whose handedness is preferably absorbed. The appearance of nested bandgaps of both handednesses during the sorting mixed chiral process is also obtained. This suggests the design of chemically controlled optical filters and optically monitored chiral pumps.
The static properties of equilibrium polymer melts confined in ultrathin films are studied by means of Monte Carlo simulations of a lattice model: the bond fluctuation model. In this work we focus on the effects of ultrathin film confinement between two parallel and neutral walls on chain size and molecular weight distribution. We compare our numerical results to analytical calculations by Semenov and Johner [Eur. Phys. J. E, 12, 469 (2003)] which predicted for ultrathin films, logarithmic corrections to the leading mean-field behavior. Our simulation data are compatible with the theoretical results.

**10:24AM U25.00013 Promotion of the Polyfluorene Beta-Phase: A First Principles Study**

ELIZABETH M. LUPTON, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City UT-84122; DAVID G. PRENDERGAST, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley CA-94720

Two configurations of polyfluorenes - potentially important for their blue emission properties in organic devices - have been identified in single molecule spectroscopy experiments: a glassy phase with random torsional angles between fluorene units, and a planar beta-phase. The twisted conformation is known to be the lowest energy structure, and the factors which promote the stabilization of the beta-phase are unclear. We present a density functional theory study of ways in which polyfluorenes could be manipulated to favor the formation of the photosynthetically more stable beta-phase. Extension along the molecular axis, which increases the stability of the planar conformation relative to the glassy phase, and the role of side groups are examined in fluorene oligomers and a polyfluorene infinite in the molecular axis. Implications for excited state properties, including fluorescence, will be discussed in the context of these results.

Supported by: The University of Utah and US DOE Contract No. DE-AC02-05CH11231

**10:36AM U25.00014 Atomic structures and electronic properties of poly(3-hexyl thiophene) on ZnO(110-1) surface.**

SEFA DAG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The atomic structures of adsorbed poly(3-hexyl thiophene) (P3HT) polymers on the non-polar ZnO surface (110-1) are studied with molecular dynamics using ab initio adjusted atomic force fields, and the electronic structures of the resulting systems are studied with direct ab initio calculations. We investigated different P3HT attachment orientations on the ZnO surface. We also studied the influence of the crystallization among the P3HT polymers to the polymer-ZnO attachment. We found that the strength of the attachment depends strongly on the P3HT crystal orientation, and to the partial charge of the surface Zn, O atoms and the end atoms of the P3HT. We studied the temperature dependence of the attachment, and the effects of the details of the attachment atomic structures to the electronic properties of the interface. This work is supported by U.S. Department of Energy, BES, under contract No. DE-AC02-05CH11231 and it used the resource of the National Energy Research Scientific Computing Center.

**10:48AM U25.00015 Ab initio study of a promising class of copolymers for application to high-efficiency photovoltaics.**

JEAN FRÉDÉRIC LAPRADE, MICHEL CÔTÉ, Département de physique and Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — In order to achieve high power conversion efficiency in bulk-heterojunction solar cells using PCBM as electron acceptor, it is essential to identify an electron donor polymer which i) harvests the largest part of the solar spectrum and ii) shows an electronic structure appropriate to PCBM. In the last few years, different groups synthetized copolymers based on either fluorene or dibenzosilole with interesting results. This presentation will report the results of density-functional theory (DFT) and time-dependent density-functional theory (TDDFT) calculations on those copolymers and their units in order to better assess the impact of changing the fluorene's 9-atom on the electronic properties. We will focus our discussion on the interplay of the counts on the energy levels and on the oscillator strength of the oligomers. O. Ingañäs & al. Appl. Phys. A, 2004, 79, 31 N. Blouin & al., Adv. Mater., 2007, 19, 2295 P.L.T. Boudreaulet & al, Macromol. Rapid Commun., 2007, 28, 2176
8:48AM U26.00003 Oxidation of the PAH Coronene by Ozone and OH Radical. ERIN MYSAK, JARED D. SMITH, JOHN T. NEWBERG, KEVIN R. WILSON, HENDRIK BLUHM, Lawrence Berkeley National Laboratory, LAWRENCE BERKELEY NATIONAL LABORATORY TEAM — Reactivity of the polycyclic aromatic hydrocarbon (PAH) coronene to oxidation sources ozone and OH radical is examined. To probe the extent of chemical reaction, product formation, and change in surface morphology as a function of reaction, we examine coronene, adsorbed onto various substrates, from both a surface and bulk perspective, with ambient pressure photoemission spectroscopy (APPEX) and aerosol mass spectrometry (AMS), respectively. For bulk on-line analysis, a 20nm thick layer of coronene adsorbed onto NaCl seed particles and reacted with either oxidant in a flow tube showed very little reactant conversion to product in the AMS. However, surface analysis by the APPEX of the same reaction where coronene was adsorbed onto model substrates showed up to 50 per cent conversion of the carbon species to oxidized carbon, depending on coronene layer thickness (about 1.5-14Å). Data obtained with these complimentary techniques provide evidence for a surface selective reaction.

9:00AM U26.00004 Morphological effects on coated aerosol kinetics. ELIAS ROSEN, EVA GARLAND, TOMAS BAER, University of North Carolina at Chapel Hill — The fate of organic material in the atmosphere can be strongly dependent on the chemical environment under which oxidation takes place. We have investigated the reaction of gas-phase ozone and oleic acid adsorbed to the surface of polystyrene latex spheres and silica aerosols to better understand how the substrate influences heterogeneous kinetics. Flow tube experiments were performed with an Aerosol Time of Flight Mass Spectrometer using a two-laser vaporization/ionization scheme to minimize analyte fragmentation. Pseudo-first-order rate coefficients suggest that ozonolysis of oleic acid proceeds differently on the hydrophobic latex and hydrophilic silica particles. Mechanistic interpretation of these results has been complicated by the discovery that the morphology of oleic acid vapor deposition onto both particle types is non-uniform, which results in the formation of discrete areas of organic material on the particle surface as evidenced by AFM and SEM/EDS measurements.

9:12AM U26.00005 Optical and microphysical properties of organic multicomponent aerosol particles. YINON RUDICH, Weizmann Institute — Atmospheric aerosols affect Earth’s climate in direct and indirect manners. The direct effect of aerosols on climate is by scattering and/or absorbing incoming solar and outgoing terrestrial radiation, which strongly modify Earth’s radiation budget. In addition, aerosols acting as cloud condensation nuclei (CCN) indirectly affect climate and precipitation by modifying the microphysical properties of clouds and cloud coverage. These climate effects depend on the chemical composition, size and morphology. We will present laboratory studies aiming at understanding how the organic component of atmospheric affect the climate system. Specifically, we present the use of cavity ring down (CRD) spectrometer to derive the extinction and complex refractive index of aerosols containing a significant organic component. By precisely measuring extinction as a function of particle size the real and imaginary refractive indices are obtained, and the single scattering albedo can be calculated. We will present results on aerosol particles containing humic like substances (HULIS). HULIS are a common component of aerosols in the atmosphere. They contribute to the CCN activity, hygroscopic properties and the density of aerosols. In addition, HULIS absorb throughout the visible range, and hence contribute to the direct climatic effect of aerosols. The absorption by organic aerosols is largely unaccounted for in models. Specifically, we will present how the absorption of aerosols containing HULIS and inorganic salts varies with wavelength, test various optical mixing rules and will present results on the extinction of core-shell particles. In addition, we will discuss how the presence of HULIS affects the surface tension of CCN at activation and of cloud droplets and its implications.

9:48AM U26.00006 Oxidation of oleic acid monolayers at air/liquid interfaces. LAURA VOSS, Bowdoin College — Field studies of marine and continental aerosols find that fatty acid films form on aqueous tropospheric aerosols. Oxidation of oleic acid monolayers by ozone was studied to understand the fate of fat-coated aerosols from both fresh and salt water sources. Using vibrational sum frequency generation spectroscopy and reflection absorption infrared spectroscopy, we present a molecular-level investigation of fatty acid monolayers at the air-water and air-sodium chloride solution interface and explore reactions with atmospheric oxidants by these model systems. Coupling sum frequency generation spectroscopy with a Langmuir trough, concurrent spectroscopic and thermodynamic data were collected to obtain a molecular picture of the monolayers. No substantial difference was observed between oxidation of monolayers spread on water and on 0.6 molar sodium chloride solutions. Results indicate that depending on the size of the aerosol and the extent of oxidation, the subsequent oxidation products may not remain at the surface of these films, but instead be dissolved in the aqueous sub-phase of the aerosol particle. Results also indicate that oxidation of oleic acid could produce monolayers containing species that have no oxidized acyl chains.

10:00AM U26.00007 Chemical and Spatial Microscopy of Individual Organic Aerosols. ALEXEI V. TVANSKI, Department of Chemistry, University of Iowa, REBECCA J. HOPKINS, MARY K. GILLES — Carbonaceous particles originating from biomass burning can account for a large fraction of organic aerosols in a local environment. Presently, their composition, physical, and chemical properties as well as their environmental effects are largely unknown. A distinct type of biomass burn particles, called “tar balls”, have been observed in a number of field campaigns, both in fresh and aged smoke. They are characterized by their spherical morphology, high carbon content and ability to efficiently scatter and absorb light. Here, a combination of scanning transmission x-ray microscopy and near edge x-ray absorption fine structure spectroscopy is used to determine the shape, structure and size-dependent chemical composition of 150 individual tar ball particles ranging in size from 0.15 to 1.2 μm. Oxygen is present primarily as carboxylic carboxyls and oxygen-substituted alkyl functional groups. The observed chemical composition is distinctly different from black carbon and more closely resembles high molecular weight humic-like substances. A detailed examination of the carbonyl intensity as a function of particle size reveals the presence of a thin oxygenated interface layer on the tar balls, indicative of atmospheric processing of biomass burn particles.

10:12AM U26.00008 OH oxidation of organic aerosols. JARED SMITH, ERIN MYSAK, MUSA AHMED, LBNL, CHRISTOPHER CAPPA, UC, Davis, STEPHEN LEONE, UC, Berkeley and LBNL, KEVIN WILSON, LBNL — Ambient aerosols play a significant role in a variety of atmospheric processes such as direct and indirect effects on radiative forcing. Chemical composition can be an important factor in determining the magnitude of these effects. However, a major fraction of organic aerosols (OA) can not be resolved on a molecular level. Recent identification of high mass oligomeric species as a major component in laboratory and ambient OA has received much attention due to the possibility that these species may account for much of the unknown organic mass in ambient aerosols. Although, a few mechanisms have been proposed, the origin and formation processes of these compounds remain largely unknown. Here we provide strong evidence for a previously unidentified mechanism of extremely rapid oligomer formation, via OH radical initiated oxidation of OA. This process appears capable of converting a sizable fraction of an organic particle to higher mass oligomers within a day of exposure to OH radicals at typical atmospheric concentrations. Furthermore, we have found that rapid volatilization is also important for specific reaction systems, and can lead to the loss of a large fraction of the particle mass. We propose that such a rapid processing is possible due to a radical chain reaction which quickly propagates throughout the entire particle and is only initiated by the surface OH reaction.

Thursday, March 13, 2008 8:00AM - 10:48AM – Session U27 DCMP: Correlated Electrons: Theory, Actinides, and Ising Systems Morial Convention Center 219
8:00AM U27.00001 Quantitative Calculation of the Spatial Extension of the Kondo Cloud . BERGMANN GERD, University of Southern California — A recently developed compact solution for the singlet state of the Friedel-Anderson and the Kondo impurity is applied to investigate the old question of a Kondo cloud in the Kondo ground state. Wilson’s states with an exponentially decreasing frame of energy cells towards the Fermi level are used. The Wilson states are expressed as free electron waves with a linear dispersion and integrated over the width of their energy cells. For the magnetic state of the Friedel-Anderson impurity one finds essentially no spin polarization in the vicinity of the d-imurity. However, for intense magnetic fields the electron spin (magnetization) becomes not only a function of the d-electron component but also of the f-electrons. The spatial range of the correlation effect of the f-electron spin is investigated in detail for the Kondo impurity. The range is inversely proportional to the Kondo energy \( \Delta K \). The extent of the electron density in real space is a detector for a resonance in energy. The spatial extension \( \xi \) and the resonance width \( \Delta \) are reciprocal and given by the relation \( \Delta \approx \hbar v \epsilon \).

8:12AM U27.00002 Perturbative Cumulant Monte Carlo Study of LiHoF\(_4\) in a Weak Transverse Magnetic Field . S.M. ALI TABELI, MICHEL GINGRAS, University of Waterloo, YING-JER KAO, Theoretical Sciences, National Taiwan University, TARAS YAVORSKII — Results from a recent quantum Monte Carlo (QMC) study of the LiHoF\(_4\) ising magnetic material in an applied transverse magnetic field \( B_z \) show a discrepancy with the experimental results, even for small \( B_z \) where quantum fluctuations are small. This discrepancy persists asymptotically close to the classical ferromagnet to paramagnet phase transition. We numerically investigate and compare this behavior with the similar diagram of LiHoF\(_3\) in the regime of weak \( B_{\|} \). In this regime, we numerically determine the effective magnetic field \( B_{\|} \) which incorporates perturbatively the small quantum fluctuations in the vicinity of the classical phase transition at \( B_{\|} = 0 \). Via this effective classical Hamiltonian, we study the \( B_{\|} - T \) phase diagram via classical Monte Carlo simulations. In particular, we investigate the influence of various effects that may be at the source of the discrepancy. We also show how our method can be generalized to numerically study the diluted LiHo\(_{1-x}\)F\(_3\) in the small \( B_{\|} \) regime.

8:24AM U27.00003 A New Heavy Fermion Compound Yb\(_3\)Pt\(_4\)\(^+\). MARCUS BENNETT, Stony Brook University, PETER KHALILFAR, DAMIRY SOKOLOV, YIUI YUEN, MOOSUNG KIM, CARL HENDERSON, WILLIAM GANNON, MEIGAN ARONSON — We report the synthesis of single crystals of a new binary heavy fermion system, Yb\(_3\)Pt\(_4\). Magnetic susceptibility measurements find Yb\(_3\)Pt\(_4\) local moment behavior above 150 K. Heat capacity measurements find a large weakly first order anomaly at 2.4 K, and the associated entropy indicates that magnetic order emerges from a doublet ground state. Magnetic field suppresses both the magnitude of the anomaly and the temperature at which the anomaly occurs, mapping out a first order phase line that ends at a tri-critical point, 1.75 T, 1.3 K. A weak cusp in the AC magnetic susceptibility indicates antiferromagnetic ordering. Above 0.2 T, the cusp becomes a step, which increases in height with increasing field indicating ferromagnetic order. The electrical resistivity of Yb\(_3\)Pt\(_4\) is that of a good metal, and the quadratic temperature dependence of a Fermi liquid is found throughout the antiferromagnetically ordered state and continues into the high field paramagnetic state. Both the magnitude of the quadratic temperature dependence of the resistivity and of \( \gamma \) are comparable to that found in heavy fermion compounds, indicating substantial quasiparticle mass enhancement. The Sommermer-Wilson ratio approaches 30 in the ordered state, suggesting strong fermionic correlations among the quasiparticles.

1Work at Stony Brook performed under NSF-DMR 0405961.

8:36AM U27.00004 Pressure and magnetic field effects in heavy-fermion UC\(_{1.5}\)Al\(_{1.5}\). A. ALSMADI, Physics Department, the Hashemite University, Jordan, H. NAKOTTE, Physics Department, NMSU, Las Cruces, NM, V. ZAPF, F. FABRIS, T.D. DIDN, A. LACERDA, NHMF, LANL, Los Alamos, NM, J. KAMARAD, Institute of Physics, CAS, Czech Republic — UC\(_{1.5}\)Al\(_{1.5}\) crystallizes in the hexagonal CaC\(_2\) structure and is described as a heavy fermion, which shows non-Fermi liquid behavior [1]. Here, we report on electrical resistivity, magnetic susceptibility, and magnetization results on polycrystalline UC\(_{1.5}\)Al\(_{1.5}\). The resistivity was measured under hydrostatic pressure up to 10kbar and in fields up to 18T. At ambient pressure and in zero field, the resistivity shows an anomaly at \( T_1 \approx 19K \) and then it goes through a maximum at \( T_{\text{max}} \approx 2K \). These two anomalies were also observed in the susceptibility data. The anomaly in the resistivity at \( T_1 \) goes to lower values with increasing fields and disappear at fields about 12T. \( T_{\text{max}} \) on the other hand goes to higher values with increasing fields. We find relatively weak pressure dependence, where both \( T_1 \) and \( T_{\text{max}} \) go down with increasing pressure. In the field scan at 2K and at ambient pressure, we find a change in the slope of the magnetoresistance at about 6.9T. Application of pressure causes a reduction of the magnetoresistance effect.


8:48AM U27.00005 Optical spectra of the heavy fermion uniaxial ferromagnet UGe\(_2\). VIOLETA GURITANU, PETER ARMITAGE, RICCARDO TEOLESI, SIDDHARTH SAXENA, ANDREW HUXLEY, DIRK VAN DER MAREL, DPMC, UNIVERSITY OF GENEVA, 24, TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, COLLABORATION, DEPARTMENT OF PHYSICS, CAVENDISH LABORATORY, COLLABORATION, DEPARTMENT DE RECHERCHE FONDAMENTALE SUR LA MATIERE CONDENSEE - SPSMS, COLLABORATION — We report on a detailed study of UGe\(_2\) single crystalline material using infrared reflectivity and spectroscopic ellipsometry. The optical conductivity suggests the presence of a low frequency interband transition ( ~300 cm\(^{-1}\)) and a narrow free-carrier response with strong frequency dependence of the scattering rate and effective mass. We observe sharp changes in the (300 cm\(^{-1}\)) low frequency mass and scattering rate below the upper ferromagnetic transition \( T_C \). They recover their unrenormalized value above \( T_C \) and for \( \omega > 250 \text{ cm}^{-1} \). In contrast no sign of an anomaly is seen at \( T_C \approx 30K \), which is the lower transition of unknown nature. These observations are consistent with the weak anomaly observed at \( T_C \) in transport and thermodynamic experiments.

9:00AM U27.00006 Ferromagnetism of Silicon Doped with Uranium Investigated to Extremes of Magnetic Field (Beyond 100 tesla). CHARLES MIELEKE, MPA-NHMF, Los Alamos National Laboratory, JASON COOLEY, WILLIAM HULTS, MST-6, Los Alamos National Laboratory — The ferromagnetic (FM) phase of Si:U \( x \times A t \% \) (where \( x \approx 0.25, 0.5, 0.75, 1.0, \) and 50.0 (i.e. US)) were studied in high magnetic fields as a function of temperature and U concentration. The effect of doping U into Si is investigated using a vis a vis the FM transition temperature (127K for \( x = 50.0 \)) and high magnetic field saturation is discussed. The effect of the FM transition temperature is approached from the point of view of correlation effects in f-electron systems. Attention to the high magnetic field saturation is investigated as it is unusually high in the \( x = 50.0 \) intermetallic compound. Ultra-high fields extending to 185 tesla is reported for the system. Issues with homogenization of the dilute samples are presented as well.

3This work was funded by LANL-LDRD20070013DR

9:12AM U27.00007 Electronic Structure of Actinide Materials 1. J.J. JOYCE, Los Alamos National Laboratory, T. DURAKIEWICZ, K.S. GRAHAM, D.P. MOORE, L.A. MORALES, J.M. WILLS, R.L. MARTIN, J.-X. ZHU, E.L. ROY, C.G. OLSON, Ames Laboratory, USDOE, G.E. SCUSERTIA, I.D. PRODAN, Rice University — Photoelectron spectroscopy results for both metallic and insulating actinide materials are reviewed and compared against model calculations. The dual nature of S f electron characteristics is discussed for photoemission results and three different electronic structure calculations. Magnetic configurations as a means of f-electron localization are discussed for metallic materials. The photoemission results for U and Pu intermetallics are compared against mixed-level-model and dynamical-mean-field-theory calculations. The experimental results for the actinide oxide Mott insulators are compared against screened hybrid functional calculations.

1Work supported by the US DOE, Office of Science, Campaign II, and the LANL LDRD program.
9:24AM U27.00008 Effects of full Coulomb interactions on electronic structure of $\delta$-Pu. EUGENY GORELOV, TIM WEHLING, HARTMUT HAFFERMAN, ALEXANDER LICHTENSTEIN, University of Hamburg, ALEXEY RUBTSOV, Moscow State University, ALEXEY LANDA, CHRIS MARIANETTI, MICHAEL FLUSS, Lawrence Livermore National Laboratory, ALEXEY SHORIKOV, ALEXEY LUKOYANOV, MICHAEL KOROTIN, VLADIMIR ANISIMOV, Institute of Metal Physics — We used the CTQMC method for the realistic simulation of electronic properties of correlated actinides. In particular, we focus on the spectral function of $\delta$-Pu, which is described in terms of a 7-orbital $f$-impurity model interacting with a metallic bath. Our CTQMC implementation solves this model by calculating a weak coupling expansion of the partition function in the fermionic multiorbital path-integral representation and provides numerically exact results for relatively high temperature. We discussed how different terms in the full on-site Coulomb vertex affect the local density of states. The comparison of CTQMC results with only diagonal density-density like Coulomb interactions and with additional non-diagonal terms in the interaction part of the Hamiltonian related with so-called spin flips terms shows the importance of the full rotationally invariant Coulomb vertex on the electronic structure of $\delta$-Pu. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:36AM U27.00009 First-principles study of electronic structure and local moment interactions in PuAm alloy. MYUNG JOON HAN, XUANGANG WAN, SERGEJ Y. SAVRASOV, Department of Physics, University of California, Davis — Expected to provide a clue about the origin of zero moment in the bulk phase of Plutonium, Pu$_{1-x}$Am$_x$ alloy has attracted a great attention, in which as Am ratio, $x$, increases, Pu approaches from bulk to atomic limit. To understand the electronic structure and the magnetic properties of Pu in different crystal environments, we perform fully self-consistent first-principles calculations of the PuAm system based on the density functional theory. Electronic structure strongly depends on the level of approximation for correlation effects. The exchange interactions between Pu 5f electrons and the Kondo screening strength were estimated and compared, which provide a new insight to Pu magnetism.

9:48AM U27.00010 Knight shifts around nonmagnetic impurities in a triangular lattice spin 1/2 antiferromagnet: Case of $k$-(ET)$_2$Cu$_2$(CN)$_3$. KAROL GREGOR, OLEXEI MOTRUNICH, California Institute of Technology — We study effects of nonmagnetic impurities in a spin-1/2 frustrated triangular antiferromagnet with the aim of understanding the observed broadening of $^{13}$C NMR lines in the organic spin liquid material $k$-(ET)$_2$Cu$_2$(CN)$_3$. For high temperatures down to $J/2$, we calculate local susceptibility near a nonmagnetic impurity, and we find a broadening of the Knight shift decays to the uniform one very quickly (few lattice spacings), and with the suggested density of impurities would not explain the observed line broadening present already at elevated temperatures; more extended defects and/or longer-ranged interactions are probably needed. At low temperatures, we assume a gapless spin liquid with a Fermi surface of spinons. We calculate the local susceptibility in the mean field and also go beyond the mean field by Gutzwiller projection. Here the Knight shift decays with a power law and oscillates at $2k_F$. However, with single site impurities the results fall short of the observed inhomogeneous broadening, calling for a better understanding of the appropriate models for the spins and impurities and of the possible ground states that are probed by such experiments.

10:00AM U27.00011 Excitons in the 1D Hubbard Model: a Real-Time Study. KHALED AL-HASSANIEH, Los Alamos National Laboratory, ADRIAN FEIGUIN, The University of Maryland, FERNANDO REBOREDO, IVAN GONZÁLEZ, ELBIO DAGOTTO, Oak Ridge National Laboratory — We study the real-time dynamics of a pair hole/doubly-occupied-site, namely a holon and a doublon, in a 1D Hubbard insulator with on-site and nearest-neighbor Coulomb repulsion. Our analysis shows that the pair is long-lived and the expected decay mechanism to underlying spin excitations is actually inefficient. For a nonzero inter-site Coulomb repulsion, we observe that part of the wave-function remains in a bound state. Our study also provides insight into the holon-doublon propagation in real space. Due to the one-dimensional nature of the problem, these particles move in opposite directions even in the absence of an applied electric field. The potential relevance of our results to solar cell applications is discussed.

10:12AM U27.00012 Investigation of Dipole-Forbidden $d-d$ Excitations in Strongly Correlated Transition-Metal Oxides Using Higher-Order Multipole, Non-resonant Inelastic X-Ray Scattering. B.C. LARSON, J.Z. TISCHLER, ORNL, C.-L. YEH, Tamkang Univ., Taiwan, C.-C. LEE, WEI KU, BNL — We have shown that quadrupole and higher order multipole non-resonant inelastic x-ray scattering (NIXS) at large wavevectors, $q$, provides direct access to dipole-forbidden $d-d$ excitations (Larson et al. Phys. Rev. Lett. 99, 026401 (2007)). NIXS measurements using the XOR/UNI beamline at the APS have shown that the large-intensity of on-site excitons in NiO and CoO is highly anisotropic in $q$ and dominates the energy loss spectrum. Energy-resolved Wannier function analyses have shown that the anisotropies, including a nodal direction for NiO, provide direct information on the point-group symmetry of the particle-hole wave functions for transition-metal oxides. The interpretation of these large-$q$ NIXS measurements will be discussed in connection with energy-resolved Wannier function analyses and LDA+$U$ dynamical response calculations. Implications for the extension of such investigations to manganite systems will be considered.

3Research sponsored by the DOE-BES Division of Materials Sciences and Engineering; the APS is supported by the DOE Office of Science.

10:24AM U27.00013 Exact many-electron ground states on the diamond Hubbard chain. ZSOLT GULACSI, Department of Theoretical Physics, University of Debrecen, Debrecen, Hungary, ARNO K AMPF, DIETER VOLLHARDT, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, Augsburg, Germany — Exact ground states of interacting electrons on the diamond Hubbard chain in a magnetic field are constructed which exhibit a wide range of properties such as flat-band ferromagnetism, correlation induced metallic, half-metallic, or insulating behavior [1]. In particular, the properties of these ground states can be tuned by changing the magnetic flux, local potentials, or electron density. The results show that the studied simple one-dimensional structure displays remarkably complex physical properties. The virtue of tuning different parameters points to new possibilities for the design of electronic devices which can switch between insulating or conducting and metallic bath. Our CTQMC implementation solves this model by calculating a weak coupling expansion of the partition function in the fermionic multiorbital path-integral representation and provides numerically exact results for relatively high temperature. We discussed how different terms in the full on-site Coulomb vertex affect the local density of states. The comparison of CTQMC results with only diagonal density-density like Coulomb interactions and with additional non-diagonal terms in the interaction part of the Hamiltonian related with so-called spin flips terms shows the importance of the full rotationally invariant Coulomb vertex on the electronic structure of $\delta$-Pu. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:36AM U27.00014 Phonon effect on elementary excitations in one-dimensional Mott insulators. HIROKO MATSUEDA, Sendai National College of Technology, AKIHIRO ANDO, Institute for Materials Research, Tohoku University, TAKAMI TOHYAMA, Yokohama Institute for Theoretical Physics, Kyoto University, ŠÁDAMICHI MAEKAWA, Institute for Materials Research, Tohoku University — We examine the interplay among phonons and elementary excitations in one-dimensional Mott insulators. For this purpose, we perform dynamical density matrix renormalization group calculations for the single-particle excitation and optical absorption spectra in the extended Hubbard-Holstein model. We find that the elementary excitations in the Mott insulators are quite easily modified by the phonons. In particular, the spinon branch in the single-particle excitation spectrum can be broadened, even when the phonons only couple with charge degrees of freedom. In addition, the exciton in the photoexcited state becomes polaronic, and this polaronic feature is enhanced by increasing the on-site Coulomb repulsion. We show the origins of these novel properties, and discuss implications of the present results in light of spectroscopic measurements in 1D cuprates.
A device incorporating a micromagnet exhibits a magnetic field difference between dots, allowing electrons in either dot to be addressed selectively. Experimentally and theoretically, the magnetic field dependence and absence of associated Rabi oscillations are consistent with a novel hyperfine mechanism.

Department, University of California at Santa Barbara — An all-electrical spin resonance effect in a GaAs few-electron double quantum dot is investigated.

TIAN BARTHEL


1Supported by NSA/LPS and ARO

8:12AM U28.00002 Decoherence of coupled spin qubits due to charge fluctuations1, GUY RAMON, Department of Physics, Santa Clara University, XUEDONG HU, Department of Physics, University of Buffalo, SUNY — One of the significant advantages of using the spin of quantum dot electrons as a qubit rather than their charge is their relative insolation from the environment. A number of recent works have utilized two-spin singlet and unpolarized triplet states in biased configuration to encode a logical qubit, which offer better control and coherence properties as compared with single spin states. When spin states are exchange coupled, however, they are potentially vulnerable to environmental fluctuations affecting charge qubits, since exchange coupling is electrostatic in nature. Here we carry out a quantitative calculation of the coupling between a biased two-spin qubit and a nearby charge fluctuator represented by a two-level-system (TLS), utilizing a multipole expansion up to and including the Quadrupole-Quadrupole order. The resulting coupling terms are used in a master equation formalism to study the dynamics of the open system that is formed by the spontaneous emission of the TLS coupled to the vacuum. We are thus able to provide a reliable estimate of the decoherence effects during various gate operations on the spin qubit as a function of the geometry and other characteristics of the system. Possible ways to alleviate the sensitivity of coupled spin qubits to charge fluctuations are also discussed.

1We acknowledge support from the D TO and from DARPA

2These authors contributed equally to this work

3These authors contributed equally to this work

8:24AM U28.00003 Hyperfine-mediated gate-driven electron spin resonance1, EDWARD LAIRD2, CRISTIAN BARTHEL3, EMMANUEL RASHBA, CHARLES MARCUS, Department of Physics, Harvard University, MICAH HANSON, ART GOSSARD, Materials Department, University of California at Santa Barbara — An all-electrical spin resonance effect in a GaAs few-electron double quantum dot is investigated experimentally and theoretically. The magnetic field dependence and absence of associated Rabi oscillations are consistent with a novel hyperfine mechanism. The resonant frequency is sensitive to the instantaneous hyperfine effective field, and the effect can be used to detect and create sizable nuclear polarizations. A device incorporating a micromagnet exhibits a magnetic field difference between dots, allowing electrons in either dot to be addressed selectively.

1Supported by NSA/LPS and ARO


1This work is done in collaboration with Sankar Das Sarma and supported by LPS-NSA and ARO-DTO.

2Now at the Naval Research Laboratory.
9:24AM U28.00006 Time-Reversal Symmetry and Electron Spin Relaxation of Lithium Donors in Silicon1. V.N. SMELYANSKIY, NASA Ames Research Center, A.G. PETUKHOV, South Dakota School of Mines and Technology, A.M. TYRYSKHIN, S.A. LYON, Princeton University — The exchange interaction (J-coupling) between electron spins provides a natural way to accomplish two-qubit operations in a spin-based, solid-state quantum processor. The J-coupling, because of its electrostatic (Coulombic) nature, is susceptible to charge noise in the environment, and hence turning on the J-coupling may cause fast decoherence of the interacting spin qubits. To clarify the effect of J-coupling on spin coherence, we performed spin relaxation measurements for exchange-coupled donors in dimers and trimers randomly formed in bulk-doped natural silicon and isotopically-purified 28Si. The longitudinal relaxation time, $T_1$, for donors in exchange-coupled dimers is found to be identical to that of isolated donors at temperatures 8-15K, solely determined by a two-phonon Orbach mechanism. The transverse relaxation time, $T_2$, for dimers is even longer than that of isolated donors because of the lower density of the dimers in our samples and thus substantially reduced dipole-dipole interactions. In natural silicon containing $5\%$ 29Si magnetic nuclei, an additional decoherence results from the nuclear-induced spectral diffusion. The spectral diffusion decoherence of J-coupled dimers and trimers is also identical to that of isolated donors. We conclude that J-coupling does not induce any additional decoherence in bulk donors in Si. However, the situation may change for donor dimers placed closer to the surface where more charge noise is expected. Supported by LPS/ARO.

9:36AM U28.00007 Spin relaxation of exchange-coupled donors in silicon. A.M. TYRYSKHIN, S. SHANKAR, S.A. LYON, Princeton University — The exchange interaction (J-coupling) between electron spins provides a natural way to accomplish two-qubit operations in a spin-based, solid-state quantum processor. The J-coupling, because of its electrostatic (Coulombic) nature, is susceptible to charge noise in the environment, and hence turning on the J-coupling may cause fast decoherence of the interacting spin qubits. To clarify the effect of J-coupling on spin coherence, we performed spin relaxation measurements for exchange-coupled donors in dimers and trimers randomly formed in bulk-doped natural silicon and isotopically-purified 28Si. The longitudinal relaxation time, $T_1$, for donors in exchange-coupled dimers is found to be identical to that of isolated donors at temperatures 8-15K, solely determined by a two-phonon Orbach mechanism. The transverse relaxation time, $T_2$, for dimers is even longer than that of isolated donors because of the lower density of the dimers in our samples and thus substantially reduced dipole-dipole interactions. In natural silicon containing $5\%$ 29Si magnetic nuclei, an additional decoherence results from the nuclear-induced spectral diffusion. The spectral diffusion decoherence of J-coupled dimers and trimers is also identical to that of isolated donors. We conclude that J-coupling does not induce any additional decoherence in bulk donors in Si. However, the situation may change for donor dimers placed closer to the surface where more charge noise is expected. Supported by LPS/ARO.

9:48AM U28.00008 Solid state quantum memory using the $^{31}$P nuclear spin. J.J.L. MORTON, Oxford University, A.M. TYRYSKHIN, S. SHANKAR, Princeton University, A. ARDAVAN, Oxford University, T. SCHENKEL, J.W. ÄGER, Lawrence Berkeley National Lab, S.A. LYON, Princeton University — Nuclear spins benefit from long coherence times compared to electron spins, but are slow to manipulate and suffer from weak thermal polarisation. A powerful model for quantum computation is thus one in which electron spins are used for processing and readout while nuclear spins are used for storage. Here we demonstrate the coherent transfer of an electron spin superposition to the nuclear spin using a combination of microwave and radiofrequency pulses applied to $^{31}$P donors in a passively-cooled pure $^{28}$Si crystal. The state is left in the nuclear spin on a time scale long compared with the electron $T_2$ and then coherently transferred back to the electron spin, thus demonstrating the $^{31}$P nuclear spin as a solid-state quantum memory. The transfer fidelity is about 84% each way, attributed to imperfections which could be corrected using composite pulses [J.J.L. Morton et al., Phys Rev Lett 95, 200501 (2005)]. Varying the time for which the state is stored in the nuclear spin permits the direct measurement of the nuclear spin $T_2$, which we have studied in the range 6.5 to 10 K.

1Supported by LPS/ARO, QIPIRC, the U.S. D.O.E. under Contract No. DE-AC02-05CH11231 and St. John’s College, Oxford

10:00AM U28.00009 Detection of low energy single ion impacts in silicon transistors. CHRISTOPH WEIS, ARUNABH BATRA, STEFANO CABRINI, LBNL, JEFFREY BOKOR, CHEUK LO, UC Berkeley, THOMAS SCHENKEL, LBNL — We report a technique for single ion doping of field effect transistors through monitoring of changes in the source-drain currents at room temperature [1]. Implant apertures are formed in the interlayer dielectrics and gate electrodes of planar, micro-scale transistors by electron beam assisted etching. Device currents increase due to the generation of positively charged defects in gate oxides when ions (121Si12+, 14+, Xe6+; 50 to 70 keV) impinge into channel regions. Implant damage is repaired by rapid thermal annealing, enabling iterative cycles of device doping and electrical characterization. We discuss integration of single ion doping for the development of silicon based quantum computer structures with donor electron and nuclear spin qubits. [1] A. Batra et al., Appl. Phys. Lett. 91, 193502 (2007)

1Supported by the National Security Agency, and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

10:12AM U28.00010 Real-time decoherence of hyperfine-coupled electrons in quantum dots. JORDAN KRYIAKIDIS, JEAN-MARC SAMSON, Dalhousie University, Halifax, Canada — We approach the study of the electron spin decoherence due to the Fermi contact hyperfine interaction with the density matrix formalism of quantum relaxation. We consider an s-type electron in the ground state of a quantum dot interacting with a thermal distribution of nuclear spins. We directly compute the time dependence of the reduced density matrix by solving the system of integro-differential equations resulting from the Liouville equation at the Born (but not Markov) approximation. We show how the spin precession can, under certain circumstances, slow down and even reverse its rotation sense.

10:24AM U28.00011 Coupling of Mechanical Modes and Shot Noise in a Radio Frequency Quantum Point Contact. J. STETTENHEIM, FENG PAN, Dartmouth College, Z. JI, Rice University, MUSTABA BAL, W.W. XUE, Dartmouth College, MADHU THALAKULAM, Rice University, L.N. PFEIFFER, K.W. WEST, Bell Laboratories, Lucent Technologies Inc., Murray Hill, NJ 07974, A.J. RIMBERG, Dartmouth College — Interesting interactions exist between the electrical and mechanical degrees of freedom in GaAs quantum nanostructures due to the piezoelectric nature of the substrate. Here, we report measurements in radio-frequency quantum point contacts (RF-QPCs) in which the photon assisted tunneling is mediated by a piezoelectric substrate. The RF-QPC has a unique ten-fold (near) degeneracy which is only slightly lifted by stresses, magnetic field and spin-orbital interaction. Despite this degeneracy, we predict, on the basis of the time-reversal symmetry and weakness of the umklapp phonon processes, an extraordinarily long relaxation time for lithium donor electron spin for the temperatures below 0.3 K. Strong temperature dependence of the spin relaxation time is due to activation-type processes with several activation exponents. Experimentally observed traces of magnetization reversal and longitudinal spin relaxation times at $T = 2.1$ K and $\alpha = 4.5$ K are in remarkably close agreement with the theory.

1Supported by ARO, NSF, and LPS/NSA.
10:36AM U28.00012 Intrinsic noise measurement of an ultra-sensitive radio-frequency single electron transistor1, W.W. XUE, Dartmouth College, Z. JI, Rice University, FENG PAN, A.J. RIMBERG, Dartmouth College — The radio-frequency single electron transistor (rf-SET) has been the focus of intense interest since its invention in 1998[1]. Using cryogenic ultra-thin film evaporation techniques [2] and an improved on-chip superconducting matching network [3], we have consistently fabricated rf-SETs with charge sensitivity of 1.7–5µe/√Hz and uncoupled energy sensitivity 1.1–5.1µe/√Hz. Using our 1GHz resonant circuit, intrinsic noise in the SET arising from a dc voltage bias was measured in the white noise limit. We measured the offset charge dependence of the intrinsic noise in the vicinity of the Josephson-quasiparticle and double Josephson-quasiparticle transport cycles. In regions for which the offset charge and resistance noise are strongly suppressed, we can determine the SET shot noise in the sup-gate regime. We discuss the effects of correlations between charge carriers on the measured Fano factor. [1] R.J. Schoelkopf et al., Science 280,1238 (1998); [2] N.A.Court et al., Cond-mat 0706.4150 (2007); [3] W.W.Xue et al., Appl.Phys.Lett. 91, 093511 (2007).

1This work was supported by NSF, ARO and LPS/NSA.

10:48AM U28.00013 Coherent electron-phonon states in suspended quantum dots: decoherence and dissipation effects1, LUIS G.C. REGO, Univ. Fed. Santa Catarina, Department of Physics — The dynamics of coherent electron-phonon (el-ph) states is investigated for a suspended quantum dot structure. Exact quantum dynamics calculations reveal that electron and phonons (comprising a thermal bath) couple quantum mechanically to perform coherent oscillations with periods in the range of tens of nanoseconds, despite the finite temperature of the phonon bath. Mechanical energy dissipation due to clamping loss is taken into account in the calculations. Although the lifetime of the coupled el-ph states decreases with the temperature, well defined Rabi oscillations are obtained for temperatures up to 100 mK. The dynamics of the coupled electron-phonon state is susceptible to various forms of external control. For instance, a weak external magnetic field can be used to control the dynamics of the system, by decoupling the electron from the phonon bath. The results cast light upon the underlying physics of a yet unexplored system that could be suitable for novel quantum device applications.

1The author acknowledges financial support from CNPq/Brazil as well as a generous allocation of computer time from CENAPAD/Campinas and NACAD/COPPE in Brazil.
9:24AM U29.00006 Mesoscopic valley-Hall effect in graphene, JOHAN NILSSON, Leiden University — An intriguing property of graphene is the existence of a degree of freedom associated with the two inequivalent valleys in the Brillouin zone. A controlled manipulation of this degree of freedom may potentially be used in novel electronic devices. We study the mesoscopic valley-Hall effect that may provide a route toward the desired control. The effect appears when the inversion symmetry of the crystal is broken, and it can generate a transverse valley current in response to an applied electric field. We look at a few sample setups and discuss the dependence on the geometry and the appearance of valley-Hall edge states. We also compare and contrast our results with those obtained from linear response theory in bulk samples.

9:36AM U29.00007 Electronic screening in graphite, JAMES REED, YOUNG IL JOE, PETER ABBAMONTE, University of Illinois at Urbana-Champaign — Nonlocal screening in highly-oriented pyrolytic graphite was investigated with inelastic x-ray scattering. Measurements were performed over a sufficiently broad range of momentum and energy to permit complete inversion of the loss function, \(-Im[\epsilon(k, \omega)]\), allowing real-time, microscopic imaging of the induced electron density around a charged impurity. In addition, we found evidence for a sign change in the zero-frequency dielectric function, \(\epsilon(k, 0)\), over a sizeable range of momentum. This “antiscreening” should cause the Coulomb interaction to be attractive, perhaps assisting superconductivity in this system.

1Funded by the Office of Basic Energy Sciences, US Department of Energy, DE-FG02-07ER46459

9:48AM U29.00008 Band Structure of K(2x2) on graphene, JESSICA MCCHESEY, AARON BOSTWICK, TAISUKE OHTA, Lawrence Berkeley National Laboratory, THOMAS SEYLLER, K.V. EMTSEV, Universitt Erlangen-Nnber, KARSTEN HORN, Fritz Haber Institute, ELI ROTENBERG, Lawrence Berkeley National Laboratory — The electronic structure of K(2x2) on graphene, the same stochiometry as bulk KC8, was studied using angle-resolved photoemission spectroscopy (ARPES). In addition to bands derived from the graphene \(\pi\) states an intercalant induced “interlayer band” is observed centered at \(\Gamma\). Of these two bands, the dominant mass renormalization occurs in the \(\pi\)-derived bands, as determined by characterization of the “kinks” in the dispersion measured by ARPES. This suggests that the superconductivity in bulk KC8 has a more important role than the interlayer band.

10:00AM U29.00009 Coulomb scattering and transport in graphene1, DMITRY NOVIKOV, Yale University — The exact transport cross-section off a Coulomb impurity in graphene [1] is proportional to the carrier wavelength. Unexpectedly, the relativistic Coulomb scattering also exhibits a pronounced attraction-repulsion asymmetry [1,2]. Massless carriers are scattered more strongly when they are attracted to a charged impurity than when they are repelled from it. This finding, confirmed recently [3], can be used to separately determine the surface density of donors and acceptors in a graphene monolayer [2]. I will outline quantitative and qualitative differences between the exact result [1] and the commonly used Born approximation for charged impurity scattering. [1] D. S. Novikov, arXiv:0706.1391, Phys. Rev. B (in press); [2] D. S. Novikov, Appl. Phys. Lett. 91, 102102 (2007); [3] J. H. Chen, C. Jang, M. S. Fuhrer, E. D. Williams, M. Ishigami, arXiv:0708.2408v2.

1Work supported by NSF Grants DMR 02-37296 and 04-39026, and by DOE Grant DE-FG02-06ER46310

10:12AM U29.00010 Resonance Raman investigation of monolayer and bilayer graphene, MARCOS PIMENTA, LEANDRO MALARD, DANIELA MAFRA, JULIANA BRANT, DANIEL ELIAS, Departamento de Fisica, UFMG, Brazil, GEORGII SAMSONIDZE, Berkeley University, JOHAN NILSSON, ANTONIO CASTRO NETO, Boston University, FLAVIO PLENTZ, ELMO ALVES, Departamento de Fisica, UFMG, Brazil — The Raman spectra of graphene samples exhibit a band around 2700 cm\(^{-1}\), the so called G’ band, that is ascribed to a double resonance Raman process involving electrons and phonons in the vicinity of the Dirac point. A dispersive behavior in the position and shape of this band is observed when we change the laser energy used in the Raman experiment, showing that it can be used to probe experimentally the dispersion of electrons and phonons near the Dirac point of graphene. We will present a resonance Raman investigation of monolayer and bilayer graphene using many different laser lines in the visible and near IR range. By the analysis of the dispersive behavior of the G’ band we can obtain information about the electronic structure of monolayer and bilayer graphene, such as the intralayer and interlayer tight-binding parameters. Our results reveal a significant asymmetry between the electronic dispersion in the valence and conduction bands of bilayer graphene. We are also able to obtain experimental values for the velocity of the TO and LA phonons near the Dirac point of graphene.

10:24AM U29.00011 Effect of contact induced states on minimum conductivity in graphene, ROKANSA GOLIZADEH-MOJARAD, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN-47906, USA — Recent experiments show that the conductivity of graphene tends to a minimum value in the range of \(~2-12\Omega^{-1}\) as the Fermi energy \(E_F\) approaches the charge neutral Dirac points \((E = 0)\). We point out that contact induced states can help explain the structure dependence of the minimum conductivity observed experimentally even if the samples were purely ballistic. Contact induced states are similar to the well-known metal induced gap states (MIGS) in metal-semiconductor Schottky junctions, which typically penetrate only a few atomic lengths into the semiconductor, while the depth of penetration decreases with increasing band gap. However, in graphene we find that these states penetrate a much longer distance of the order of the width of the contacts. As a result, ballistic graphene samples with a length less than their width can exhibit a resistance proportional to length that is not ‘Ohmic’ in origin, but arises from a reduced role of contact-induced states. While actual samples are probably not ballistic and involve scattering processes, our results show that these contact induced effects need to be taken into account in interpreting experiments and minimum conductivity depends strongly on the structure and configuration (two- vs. four-terminal).

10:36AM U29.00012 Theory of superconductivity by the edge states in graphene, KEN-ICHI SASAKI, MASAHIRO SUZUKI, RICHIRO SAITO, Tohoku University — Superconductivity in graphite intercalation compound and carbon nanotubes has been attracting much attention due to its high superconducting transition temperature above 10 K. However, the density of states (DOS) near the Fermi level of graphene is not sufficient to explain the observed high transition temperature. Thus, the mechanism of the superconductivity is an important issue. The STS measurements (Kobayashi et al., PRB73.125415, Niihi et al., PRB73.085421) show an anomalous DOS near the Fermi level of graphene which is relevant to localized edge states. The edge states significantly enhance the local DOS near the zigzag edge. Thus, it is valuable to examine the effect of the edge states on the superconductivity. Using the Eliashberg equation, we obtain an appreciable transition temperature for the edge states. We found that the effects of the Coulomb interaction and Fermi energy position are sensitive to the formation of superconducting gap. We will discuss the condition for observing the edge state superconductivity. (Sasaki et al., J. Phys. Soc. Jpn. 76, 033702 (2007))
10:48AM U29.00013 Ground-state carrier density in graphene, ENRICO ROSSI, SANKAR DAS SARMA, Condensed Matter Theory Center, University of Maryland, College Park, MD 20742-4111, USA — We calculate the carrier density spatial distribution for the ground state of a single layer graphene sheet in presence of randomly distributed charged impurities. In our calculation we include the effects due to the exchange and correlation energy. We carefully study how the distance $d$ of the charge impurities from the graphene layer and an external bias affect the spatial distribution of the carrier density. At zero bias we find that the carrier density is characterized by the presence of electron and hole puddles with equal probability and that, for $d \approx 1$, the typical size of the puddles is of the order of 30 nm in agreement with recent experiments. With the same approach we study the situation when a tunable barrier potential is applied locally and a bipolar junction within the graphene sheet is formed. This work is supported by NRI-NSF.

8:00AM U30.00001 Ab-initio study of polarization in graphene films, ERIC YU, Department of Electrical and Computer Engineering, Cornell University, DEREK STEWART, Cornell Nanoscale Facility, Cornell University, SANDIP TIWARI, Department of Electrical and Computer Engineering, Cornell University — We present an ab-initio analysis of polarization of multilayer graphene systems under applied electric fields. The effects of applied electric fields are calculated using a Berry phase approach with a plane-wave density functional formalism. We have determine polarization values for graphene films and carbon nanotubes and find that the polarizability of graphene films follows a linear relationship with the number of layers. We also examined changes in the induced charge distribution as a function of graphene layers. We focus in particular on bilayer graphene and find that the induced charge accumulates primarily on the B sublattice sites. This induced charge distribution was also confirmed by a separate tight-binding Green’s function calculation.

8:12AM U30.00002 Large-Scale Self-Consistent Simulation of Multilayered Graphene Devices, DENIS ARESHKIN, BRANISLAV K. NIKOLIC, University of Delaware — We use the Density Functional Theory-based Self-Consistent Environment-Dependent Tight-Binding (SC-EDTB) and self-consistent Non-equilibrium Green function formalism (NEGF) to test the all-graphene multilayer circuit concept. The key element of multi-layered circuits, which is to become available through high-speed graphene research, is the highly perforated graphene layer. The latter serves as an electrical insulator due to its relatively large band gap, and poor ballistic coupling to the conductive parts of the circuit. High bias $V − V'$ characteristics for various normally-on and normally-off transistor configurations were simulated, and transistor tolerance to manufacturing defects and imperfections was tested. The usage of SC-EDTB-NEGF makes it possible to model quantum transport through realistic devices composed of large number of carbon atoms ($\sim 10^6$), which are within the reach of presently available processing techniques. Other circuit elements, such as electric interconnects between different layers, wires crossings, and electric interconnects within the same layer are also considered.

8:24AM U30.00003 Energy bands of multilayer graphenes, WEN-YING RUAN, JIA-AN YAN, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology — The energy bands of L-graphene have been obtained using first-principles calculations. We found that after the introduction of interlayer coupling the linear valence and conduction bands of isolated layers can either remain or develop into parabolic bands or bands with a very flat top(bottom), depending on the stacking geometry. A theoretical explanation and some general rules have been developed based upon the tight-binding model with only the nearest-neighbor interactions.

8:36AM U30.00004 Effect of strain on the electronic structure of graphene, EDGAR MARTINEZ, Departamento de Fisica de Aplicada, Cinvestav-Merida, Yucatan, Mexico A.P. 73 Cordemex 97310 Merida, Yucatan, Mexico, EDUARDO CIFUENTES, Facultad de Ingenieria, Universidad Autonoma de Yucatan, Mexico, ROMEO DE COSS, Departamento de Fisica de Aplicada, Cinvestav-Merida, Yucatan, Mexico — Graphene has been attracting interest due to its remarkable physical properties resulting from an electron spectrum resembling relativistic dynamics (Dirac fermions). Thus, is desirable to know methods for controlling the charge carriers in graphene. In this work, we propose that the electronic properties of graphene can be modulated via isotropic and uniaxial strain. We have studied the electronic structure of graphene under mechanical deformation by means of first principles calculations. We present results for the charge distribution, electronic density of states, and band structure. We focus the analysis on the behavior of the Dirac cones and the number of the charge carriers as a function of strain. We find that an isotropic tensile strain increases the effective mass of carriers and an isotropic compression strain decrease it. Uniaxial tensile strain induce a similar behavior, as strain increase effective mass increase. Thus, our results show that strain allows controllable tuning of the graphene electronic properties. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

8:48AM U30.00005 Band-gap engineering in graphene systems for electronic applications, SUJATA PAUL, MARCO BUONGIORNO-NARDELLI, NC State University — Ultrasound graphene films including monolayers, bilayers and graphene nanoribbons are intensely studied for the development of future electronic and optoelectronic devices. In this work we will present first principles electronic/phonon structure calculations to elucidate the role of geometry and interactions (electric field, edge functionalization, gating etc.) in the determination of the electronic properties of a wide variety of graphene systems (multi-layers, ribbons etc.). One preliminary objective of this task is to explore ways to accurately control the band gap through the careful design of the active graphitic systems. The coupling between electron and lattice dynamics will be analyzed via the evaluation of the electron-phonon coupling parameters and phonon dispersions calculations. We will discuss the growth of graphene layers on a preferred substrate e.g. SiC an Si.

9:00AM U30.00006 Effect of Disorders in Graphene Nanoribbon Field-Effect Transistors, YOUNGKI YOON, U of Florida, GIANLUCA FIORI, Università di Pisa, SEOKMIN HONG, U of Florida, GIUSEPPE IANNACCONE, Università di Pisa, JING GUO, U of Florida — Recent progress on the graphene and graphene nanoribbon (GNR) has provoked strong interests in GNR field-effect transistors (FETs) for future digital and analog nanoelectronics applications. In this work, device characteristics of GNRFETs are calculated by solving the non-equilibrium Green's function (NEGF) transport equation in an atomicistic $p^2$ orbital basis set self-consistently with three-dimensional (3D) Poisson equation. The effects of a lattice vacancy, ionized impurity, and edge roughness on transistor performance and characteristics are examined by the atomistic simulations. We show that even a single disorder can have a significant effect on the device characteristics of GNRFETs due to the atomically thin and nanometer-wide channel geometry. For example, a single lattice vacancy can affect the on-current of a GNRFET by 40%. Localized states in the GNR band gap energy range can be induced by the disorders, which affect quantum transport and self-consistent electrostatics. Significant variations between devices are expected due to disorders, but the GNRFETs still switch in the presence of moderate amount of disorders.
investigating the edge states of the Z-BGNR, we notice that the trigonal warping of the bilayer graphene sheets are reflected on in the edge state structure of the parameter bilayer graphite nanoribbons (Z-BGNR) with various ribbon width.

There exist many one-dimensional energy bands. The low energy bands are drastically changed by the interlayer atomic hoppings, such as the destruction of state degeneracy, alteration of Fermi-momentum states, creation of extra band-edge states, and modulation of energy gap. The composite systems are metals or semiconductors, which depends on the alignment and the geometry of carbon nanotube. The main characteristics of electronic structures are directly reflected in the electronic switch.

Based on this study, only the two-layer FLG is useful as a nanoscale electronic switch.

**References**


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**9:12AM U30.00007 Diluted Graphene Antiferromagnet**, HERBERT FERTIG, Indiana University, LUIS BREVY, Instituto de Ciencia de Materiales de Madrid, SANKAR DAS SARMA, University of Maryland — We study RKKY interactions between local magnetic moments for both doped and undoped graphene. We find in both cases that the interactions are primarily ferromagnetic for moments on the same sublattice, and antiferromagnetic for moments on opposite sublattices. This suggests that at sufficiently low temperatures dilute magnetic moments embedded in graphene can order into a state analogous to that of a dilute antiferromagnet. We find that in the undoped case one expects no net magnetic moment, and demonstrate numerically that this effect generalizes to ribbons where the magnetic response is strongest at the edge, suggesting the possibility of an unusual spin-transfer device. For doped graphene we find that moments at definite lattice sites interact over longer distances than those placed in interstitial sites of the lattice (1/R^2 vs. 1/R^3) because the former support a Kohn anomaly that is suppressed in the latter due to the absence of backscattering.

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**9:24AM U30.00008 Magnetization measurement of highly oriented pyrolytic graphite surface with a spin-polarized metastable helium beam**, SHIRO ENTANI, MITSUNORI KURAHASHI, YASUSHI YAMAUCHI — Magnetic ordering in nanometerscale graphic materials has attracted much interest in recent years. Some theoretical studies have predicted that the origin of ferromagnetism in these materials was attributed to defects in graphic structures, such as edges and topological defects. Employing surface analytical technique is favorable for elucidation of these predictions by experimental studies, because there exist a number of pores and steps at the graphite surface and the structure not in an equilibrium phase might be realized at a surface state. In this work, we have successfully detected the magnetization in highly oriented pyrolytic graphite (HOPG) surface using a spin-polarized metastable helium (He*) beam under high magnetic field up to 5 T. The He* beam is an extremely surface-sensitive probe and the surface magnetization can be analyzed by measuring the asymmetry of sample current induced by the He* spin direction [1]. The observed value of the asymmetry shows a clear temperature dependence and is much larger than that of magnetic impurities measured by Auger electron spectroscopy. Thus, we could conclude that this surface magnetism is an intrinsic property of the HOPG itself other than the diamagnetism.


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**9:48AM U30.00010 Band structure engineering of graphene by strain**, JIANXIN ZHONG, GUI GUI, JIN LI, Department of Physics, Xiangtan University, Hunan 411105, China — We have investigated the electronic structure of graphene under different planar strain distributions using the first principles pseudopotential plane-wave method and the tight-binding approach. We found that graphene with a symmetrical strain distribution is always a zero band gap semiconductor and its pseudogap decreases linearly with the strain strength in the elastic regime. However, asymmetrical strain distributions in graphene result in opening of band gaps at the Fermi level. For the graphene with a strain distribution parallel to C-C bonds, its band gap continuously increases to its maximum width of 0.486 eV as the strain increases. For the graphene with a strain distribution perpendicular to C-C bonds, its band gap continuously increases only to 0.170 eV. The anisotropic nature of graphene is also reflected by different Poisson ratios in different directions. We found that the Poisson ratio is 0.079 and 0.255 for the strain distributions parallel to or perpendicular to C-C bonds, respectively. These findings are important for understanding and controlling the transport properties of graphene systems.

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**10:00AM U30.00011 Electronic properties of nanotube-graphene composite carbon systems**, YEN-HUNG HO, Department of Physics, National Cheng Kung University, C.P. CHANG, Center of General Education, Tainan University of Technology, M.F. LIN, Department of Physics, National Cheng Kung University — Band structures of nanotube-graphene hybrid carbon systems are calculated by the tight-binding model. The Lennard-Jones potential is used to determine the optimal geometry for a single-walled carbon nanotube and a monolayer graphene. There exist many one-dimensional energy bands. The low energy bands are drastically changed by the interlayer atomic hoppings, such as the destruction of state degeneracy, alteration of Fermi-momentum states, creation of extra band-edge states, and modulation of energy gap. The composite systems are metals or semiconductors, which depends on the alignment and the geometry of carbon nanotube. The main characteristics of electronic structures are directly reflected in density of states. DOS exhibits a lot of asymmetric prominent peaks. The predicted results could be verified by the experimental measurements from the scanning tunneling spectroscopy.

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**10:12AM U30.00012 Edge states of zigzag bilayer graphite nanoribbons**, JUN-WON RHIM, KYUNGSUN MOON, Department of Physics, Yonsei University, Seoul, South Korea, CONDENSED MATTER THEORY GROUP TEAM — Electronic structures of the zigzag bilayer graphite nanoribbons (Z-BGNR) with various ribbon width N are studied within the tight binding approximation. Neglecting the small inter-layer hopping parameter γ_z, there exist two fixed Fermi points ±k∗ for the ribbon width with the peculiar energy dispersion near k∗ as ε(k) ~ ε(k−k∗)^N. By investigating the edge states of the Z-BGNR, we notice that the tringular warping of the bilayer graphene sheets are reflected on the edge state structure of the Z-BGNR. With the inclusion of γ_z, the two above Fermi points are not fixed, but drift toward the vicinity of the Dirac point with the increase of the width N as shown by the finite scaling method and the peculiar dispersions change to the parabolic ones.

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**Thursday, March 13, 2008 8:00AM - 11:00AM – Session U31 DMP GMAG: Focus Session: Multiferroics II: Theory and LuFe2O4**

Morial Convention Center 223
8:00AM U31.00001 Spontaneous currents and charge redistribution in Mott insulators, DANIEL KHOMSKII, Universitaet zu Koeln, LEV BULAEVSKI, CHRISTIAN BATISTA, Los Alamos National Laboratory, MAXIM MOSTOVOY, Groningen University — The standard view is that at low energies Mott insulators exhibit only magnetic properties while charge degrees of freedom are frozen out as the electrons become localized by a strong Coulomb repulsion. We demonstrate that this is in general not true: for certain spin textures spontaneous circular electric currents or nonuniform charge distribution exist in the ground state of Mott insulators. The latter can give a purely electronic mechanism of multiferroic behaviour. In addition, low-energy "magnetic" states compare to the dielectric and magnetic phenomena, leading to interesting states like the electric field-induced "ESR" transitions, rotation the electric field polarization and resonances which may be common for both functions producing a negative refraction index in a window of frequencies.

8:12AM U31.00002 First-Principles Study of Large MagnetoElectric Coupling in Triangular Lattices, KRIS T. DELANEY, Materials Research Laboratory, UC Santa Barbara, MAXIM MOSTOVOY, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, NICOLA A. SPALDIN, Materials Department, UC Santa Barbara — We investigate, using density functional theory, the magneto-electric coupling in a frustrated antiferromagnet in which the combination of frustration with magnetic interactions mediated by Anderson superexchange leads to a unconventional and large coupling between polarization and magnetic order. The nature of the superexchange mechanism can be manipulated through polarization of the lattice upon application of an electric field, leading to a strong magnetoelectric effect. We demonstrate the effect in a Mn-based triangular lattice that is closely related to the Kagomé structure, with modifications to avoid self-compensation of the induced magnetic order. For our study, we employ the VASP software package with LSDA+U for describing electron exchange and correlation effects. A fully noncollinear treatment of the spinors is essential to describe the complex spin structures that the system adopts.

8:24AM U31.00003 Trends in spin exchange interactions and ferroelectric polarization in the orthorhombic $R\text{MnO}_3$ series, SILVIA PICOZZI, KUNIHIKO YAMAUCHI, CNR-INFM L Aquila, Italy, BIPAL SANYAL, Uppsala Univ., Uppsala, Sweden, FRANK FREIMUTH, STEFAN BLÜGEL, Forschungszentrum Julich, Germany, ELBIO DAGOTTO, Oak Ridge Natl. Lab. and Univ. Tennessee, TN — Recently, magnetic ferroelectricity induced by Heisenberg-type interactions has been theoretically predicted in E-type antiferromagnetic (AFM) $R\text{MnO}_3$. In order to fully clarify this unconventional microscopic mechanism, we have studied the structural, magnetic and ferroelectric properties for the entire family of orthorhombic $R\text{MnO}_3$ ($R=$ rare earth ions), based on first-principles density functional calculations. The ferromagnetic exchange interaction between nearest-neighbor Mn sites decreases with the ionic radius of $R$ (concomitantly with the in-plane Mn-O-Mn bond angle), whereas the anti-ferromagnetic next-nearest neighbor interaction rather stays constant in the series. The competition of these exchange interactions results in a complicated magnetic phase diagram. The decrease in the Mn-O-Mn angle also affects the hopping integrals between Mn ions (as determined from Wannier functions), so that the calculated electric polarization in E-type AFM $R\text{MnO}_3$ is remarkably reduced throughout the rare earth series.

8:36AM U31.00004 First-principles study of magneto-electric coupling in TbMnO$_3$, ANDREI MALASHCHEVICH, DAVID VANDERBILT, Rutgers University — At room temperature, the perovskite TbMnO$_3$ forms an orthohombically distorted lattice with the $Pbnm$ space group. Below $\sim$27 K the magnetic moments on the Mn atoms develop incommensurate cycloidal order, and simultaneously a polarization appears. We present a first-principles study of this low-temperature phase in which the ordering of the Mn$^{3+}$ moments is forced to be commensurate in a 60-atom supercell, approximating the experimental wavevector. The calculations are based on a non-collinear spin treatment of density-functional theory in the local-density approximation, with the polarization computed using the Berry-phase technique. We confirm that the electric polarization appears only when the spin-orbit coupling is turned on. Both electronic and lattice-mediated contributions to the polarization appear, the latter being dominant. We make a normal-mode analysis of the lattice contribution and discuss the ability of a model based on local Dyzaloishinski-Moriya interactions to reproduce the computed pattern of forces.

8:48AM U31.00005 MagnetoElectric Chains: Quasi-One-Dimensional Multiferroics, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National laboratory — Recently discovered pyrochlores represent an example of a multiferroic containing quasi-one dimensional (Q1D) building blocks of zig-zag chains of edge-sharing octahedra along the c-axis of the crystal. This leads us to the natural question: what types of Q1D symmetries would allow for the simultaneous presence of polarization and magnetization? Moreover, what kinds of phase transitions can exist between two different Q1D magnetic phases? From this perspective we study quasi- one-dimensional magnetic symmetry in 3D space (magnetic rod groups), enumerate Q1D magnetic point groups that allow for magneto-electricity and illustrate their role in low-dimensional multiferroic phase transitions.

9:00AM U31.00006 Influence of oxygen defects and lattice distortions on the energy gap formation and magnetic properties of multi-ferroic materials, JUJI PULIKKOTIL, VLADIMIR ANTROPOV, Ames Laboratory — Full potential density functional calculations are performed to study the effects of O-vacancies on the structural parameters and electronic properties of $R\text{MnO}_4$ ($R=$ Y, rare-earths). We find that vacancies at the 2a-position of the hexagonal unit cell can introduce a small gap of magnitude $0.2\text{eV}$. Although significantly lower than the experimentally observed value of $2.5\text{eV}$, we claim that already such defects, which in general are inevitable in oxides, can introduce the energy gap in addition to the most commonly accepted Coulomb correlation mechanism. Besides, the off-plane O-vacancies modify the magnetic properties of the system and induce small magnetic polarization on the in-plane O-sites and at the interstitials. The electronic structure and magnetic properties modifications as a function of several lattice distortions have been analyzed. We also discuss the mechanisms of the exchange coupling and its most effective path. In addition we compare previously known results of the electronic structure calculations for these systems.

9:12AM U31.00007 Domain structure and magnetization reversal in multiferroic LuFe$_2$O$_4$, WEIDA WU, SOONYONG PARK, CHENGLIN ZHANG, S.-W. CHEONG, Department of Physics and Astronomy, Rutgers University — We report real space magnetic imaging of single crystal multiferroic LuFe$_2$O$_4$ via variable temperature magnetic force microscopy (VT-MFM). The magnetization reversal of LuFe$_2$O$_4$ is investigated in detail with MFM in magnetic fields up to 8 tesla at several temperatures below $T_N=230\text{K}$. Our results suggest that the domain structure and the magnetization reversal of LuFe$_2$O$_4$ are different from those of conventional FM magnets with a uniaxial anisotropy. These unconventional behaviors may originate from the low dimensional and the unusual spin-charge frustration of LuFe$_2$O$_4$.

9:24AM U31.00008 Interplay of charge order and magnetism in LuFe$_2$O$_4$, M. ANGST, Oak Ridge National Laboratory, Oak Ridge TN, R.P. HERMANN, Institut fuer Festkoerperforschung, Forschungszentrum Julich, Germany, A.D. CHRISTIANSSON, W. TIAN, R. JIN, B.C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge TN — Ferroelectricity in LuFe$_2$O$_4$ may originate from charge order and seems to be coupled the magnetism as well. Both charge order and magnetism, conflicting reports have been published. We have recently grown single crystals exhibiting features in magnetization sharper that previously reported and suggesting an additional transition around 175 K. Neutron scattering experiments have revealed Q1D magnetic and charge order. We will also present recent growth, characterization and magnetization measurements on these crystals, which indicate a subtle interplay of magnetism, charge order, and structural distortions. Superstructure reflections studied include (1/3,1/3,n and n/2) (exhibiting small systematic deviations away from 1/3), satellites to (0,0,3/2n) and (1/3,1/3,n and n/2), and two other types of reflections. Supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US Department of Energy.
9:36AM U31.00009 Three dimensional magnetic correlations in LuFe$_2$O$_4$. M.D. LUMSDEN, A.D. CHRISTIANSON, M. ANGST, Oak Ridge National Laboratory, Oak Ridge TN 37831, Z. YAMANI, Canadian Neutron Beam Centre, NRC, Chalk River, Canada, W. TIAN, R. JIN, S.E. NAGLER, B.C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge TN 37831 — LuFe$_2$O$_4$ has recently attracted much attention due to a novel electronically driven ferroelectric transition and concomitant indications of coupling between magnetic degrees of freedom and a large spontaneous polarization. To examine the behavior of LuFe$_2$O$_4$ in further detail, we have performed extensive polarized and unpolarized neutron diffraction experiments on high quality single crystal specimens. These measurements reveal two phase transitions involving magnetic degrees of freedom below 300 K. At 240 K we find the onset of three dimensional ferrimagnetic order. The refined ferrimagnetic spin structure is a symmetry allowed magnetic structure of the parent R-3m space group with a propagation vector of (1/3 1/3 1/3). Below 175 K many of the magnetic Bragg peaks become significantly broadened and a broad diffuse component to the magnetic scattering becomes evident. In addition, a new set of satellites is observed indexed as (1/3 ±δ 1/3 ±δ 3L/2) where δ ≈ 0.027. Polarized neutron diffraction measurements indicate that these satellites have a substantial magnetic component.

9:48AM U31.00010 Optical properties of LuFe$_2$O$_4$. XIAOSHAN XU, TATIANA BRINZARI, JANICE MUSFELDT, University of Tennessee, Knoxville, MANUEL ANGST, DAVID MANDRUS, Oak Ridge National Laboratory — We measured the optical properties of single crystalline LuFe$_2$O$_4$ as a function of temperature and compared the results with recent electronic structure calculations. The 300 K optical gap is found to be ~ 0.4 eV. The optical conductivity is very sensitive to temperature and shows a sharp transition at around 170 K structural transition. The Fe$^{2+}$ to Fe$^{3+}$ charge transfer transition (at approximately 1.5 eV) sharpens dramatically at low temperature, a trend that may be connected with the complex charge order of handedness.

1This work is supported by the U.S. Department of Energy.

10:00AM U31.00011 Effect of oxygen deficiencies on charge ordering in RFe$_2$O$_4$−δ (R=Lu and Y). Y. HORIBE, Rutgers University, S. MORI, S. SHINOHARA, Y. MATSUO, Osaka Prefecture University, N. IKEDA, Okayama University, S-W. CHEONG, Rutgers University — Charge ordering (CO) of Fe$^{2+}$ and Fe$^{3+}$ on the triangular lattice in RFe$_2$O$_4$−δ (R=Lu and Y) is suggested to play an important role in the physical properties such as ferroelectricity. Herein, we report changes in the CO structures due to the oxygen deficiencies in RFe$_2$O$_4$−δ by transmission electron microscopy. At room temperature, characteristic superlattice reflections at (1/3 1/3 1/2)-type positions can be observed in the nearly stoichiometric YFe$_2$O$_4$−δ, where the diffuse streaks along c*-axis can be seen clearly in the non-stoichiometric YFe$_2$O$_4$−δ. It is suggested that the correlations between the Fe-O bilayers are suppressed due to the oxygen vacancies and therefore the two-dimensional charge ordering appears in the non-stoichiometric samples at room temperature.

10:12AM U31.00012 Ferroelectricity in an Ising Chain Magnet. V. KIRYUKHIN, Y.J. CHOI, H.T. YI, S. LEE, S-W. CHEONG, Rutgers Univ., Q. HUANG, NIST — The concept of magnetism-driven ferroelectricity has recently drawn significant attention. Among the simplest model systems showing this effect are magnetic spiral compounds, and frustrated collinear chain magnets with alternating charge order. While many experimental realizations of the former systems exist, no undisputed examples of the latter have been reported so far. Herein, we report discovery of an experimental realization of this model in an Ising chain compound with an up- down-down magnetic order. Unlike in the spiral magnetoelectrics where antisymmetric exchange coupling is active, the symmetry breaking in this system occurs through exchange striction associated with symmetric superexchange coupling. Since the latter can be large, this observation may help identify candidate systems with large magnetoelectric coupling and significant magnetoelectric effects.

10:24AM U31.00013 Magnetoelastic effect in Cr$_2$O$_3$ thin films. XI HE, University of Nebraska-Lincoln, YI WANG, SARBESWAR Sahoo, CHRISTIAN BINEK — Magnetoelastic materials experienced a recent revival as promising components of novel spintronic devices [1, 2, 3]. Since the magnetoelastic (ME) effect is relativistically small in traditional antiferromagnetic compounds like Cr$_2$O$_3$ (max. $\alpha_{xx} \approx 4\mu m$) and also cross-coupling between ferroic order parameters is typically small in the modern multiferroics, it is a challenge to electrically induce sufficient magnetization required for the envisioned device applications. A straightforward approach is to increase the electric field at constant voltage by reducing the thickness of the ME material to thin films of a few nm. Since magnetism is known to be affected by geometrical confinement thickness dependence of the ME effect in thin film Cr$_2$O$_3$ is expected. We grow (111) textured Cr$_2$O$_3$ films with various thicknesses below 500 nm and study the ME effect for various ME annealing conditions as a function of temperature with the help of Kerr-magnetometry. [1] P. Borisov et al. Phys. Rev. Lett. 94, 117203 (2005). [2] Ch. Binek, B.Doudin, J. Phys. Condens. Matter 17, L39 (2005). [3] R. Ramesh and Nicola A. Spaldin 2007 Nature Materials 6 21.

1Financial support by NSF through Career DMR-0547887 and MRSEC DMR-0213808 and the Nebraska Research Initiative is gratefully acknowledged.

10:36AM U31.00014 First-principles approach to lattice-mediated magnetoelectric effects. JORGE IGÜNEZ, ICMAB-CSIC — I will present a first-principles scheme for the computation of the magnetoelectric (ME) response of magnetic insulators. The method focuses on the lattice-mediated part of the magnetic response to an electric field, which can be expected to be the dominant contribution in materials displaying a strong coupling, thus avoiding the technical difficulties associated to the treatment of a purely electronic ME effect. I will describe results of calculations for Cr$_2$O$_3$ and other model magnetoelastic compounds.

1Supported by MacoMuFi (STREP_FP6-03321).

10:48AM U31.00015 Chirality, Handedness and Pseudovectors. THOMAS A. KAPLAN, Michigan State University, S. D. MAHANTI, Michigan State University, KYLE WARLOW, Iowa State University — Chirality has been, to our knowledge, universally defined as a symmetry property, namely, lack of mirror symmetry of a physical object (e.g. a molecule) or, more generally, a physical situation (e.g. light propagation). It is understood that the mirror can be followed by a proper rotation and/or translation. The word chirality (Greek: hand), was added by Lord Kelvin after Pasteur noted the physical importance of right- and left-handed molecules, and, in this context, is considered identical to handedness. However, there is another context, equally important, where handedness has a different meaning, namely the handedness associated with the definition of the cross-product of two vectors. We call the former def. 1, the latter, def. 2. We show that the two meanings are essentially different by giving examples which are simultaneously handed (def. 2) and not chiral. These are drawn from light waves, spin spirals and multiferroics. Thus we show that there must be a distinction between chirality and the general idea of handedness.

Thursday, March 13, 2008 8:00AM - 11:00AM — Session U32 GMAG DMP: Focus Session: Magnetic Multilayers and Nanostructures Morial Convention Center 225
8:00AM U32.00001 Unusual resonant response in [Fe(001)/Cr(001)]10/ MgO(001) magnetic multilayers in magnetic field. VLADIMIR PRYADUN, FARKHAD ALIEV, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, Spain, ETIENNE SNOECK, Groupe NanoMateriaux, CEMES-CNRS, Toulouse, France — We report on experimental observation of unusual electromagnetic resonances in [Fe/Cr]10 multilayers epitaxially grown on MgO(001) substrates and measured by using balanced excitation and detection schemes. Electric voltage resonances with quality factor exceeding $10^3$ induce strong enhancement of Hall resistance for specific frequencies. Surprisingly, the continuum mechanics model for suspended Fe/Cr layers accounts well for the observed phenomena. Cross-sectional electron microscopy analysis of the multilayers confirms that we could be dealing with non-suspended nanoelectromechanical system.

8:12AM U32.00002 Field Dependence of the Magnetic Roughness of CoFe(B)/MgO.1. ¶ YVES IDZERDA, JOE DVORAK, EZANA NEGUSSE, ALEX LUSSIER, Montana State University, S.R. SHINDE, Y. NAGAMINE, S. FURUKAWA, K. TSUNEKAWA, D.D. DJAYAPRAWIRA, Canon-ANELVA Corporation — We have measured the field dependent roughness of the magnetic interface of CoFe and CoFeB films covered by MgO by using diffuse X-ray resonant magnetic scattering (diffuse-XRMS) of circular polarized light. The samples studied were 3.0 nm of either a Co(70)/Fe(30) or a Co(60)/Fe(20)/B(20) film covered by 1.8 nm MgO created by UHV sputtering system (ANELVA C-7100). By comparing the specular scattering map and the diffuse scattering map for a large range of incidence angles for photons resonantly tuned near the Co L3-edge as the applied magnetic field is swept through the coercive field, we have determined the chemical and magnetic roughness as a function of applied field. For the CoFeB films, the magnetic scattering of the X-rays increases significantly as the film passes through the coercive field where the magnetic in-plane correlations are relatively short range, indicating the presence of small magnetic domains during moment reversal. For the CoFeB films, there is no significant increase in magnetic scattering at the coercive field, consistent with large domain switching.

3This work supported by the Office of Naval Research.

8:24AM U32.00003 Enhanced Electronic Density of States Observed in Fe-Cr Magnetic Multilayers1. ¶ DAVID W. COOKE, FRANCES HELLMAN, Physics Dept., University of California at Berkeley, MATTHEW CAREY, Hitachi Global Storage Technologies San Jose Research Center — Magnetic multi-layer structures have garnered much interest over the past two decades particularly because of the giant magnetoresistance (GMR) effect and its application to information storage technology. Iron-chromium multi-layer structures have been studied extensively, but there remain many questions in the field due to the complex behavior of the anti-ferromagnetic layer (Cr). Using our silicon micro-machined calorimeters, we examine the low temperature specific heat for a range of sputtered MML films grown under similar conditions to those used in industry. We have observed an enhanced electronic density of states in the Fe-Cr MMLs far beyond that of the iron or chromium individually. We compare this enhancement to the observed GMR behavior through a systematic study varying the thickness of the spacer layer.

4This work was supported by the Director of the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

8:36AM U32.00004 High bias voltage effect on spin-dependent conductivity and low frequency noise in epitaxial Fe/MgO/Fe magnetic tunnel junctions. FARKHAD ALIEV, RUBEN GUERRERO, DAVID HERRANZ, RAUL VILLAR, Universidad Autonoma de Madrid, Spain, FANNY GREULLET, CORIOLAN TIUSAN, MICHEL HEHN, FRANCOIS MONTAIGNE, Nancy Universitie, France — Low temperature (10K) high voltage bias dynamic conductivity (up to 2.7V) and shot noise (up to 1V) were studied in epitaxial Fe(100)/Fe-C/MgO(100)/Fe(100) magnetic tunnel junctions, as a function of the magnetic state. The MTJs show large TMR (185% at 300K and 330% at 4K). Multiple sign inversion of the magnetoresistance is observed for bias polarity when the electrons scan the electronic structure of the bottom Fe-C interface. The shot-noise shows a Poissonian character validating the high structural quality of the MgO barrier [1]. We have found that the normalized I/f noise (Hooge factor) asymmetry between parallel and antiparallel states may strongly depend on the applied bias and its polarity. These MTJs exhibit record low Hooge factors being at least one order of magnitude smaller than previously reported [2]. [1] R. Guerrero, et al., Appl. Phys. Lett. 91, 132504 (2007); [2] F.G. Aliev, et. al., accepted to Appl. Phys. Lett.).

8:48AM U32.00005 Giant Magnetoresistance in Nanoparticulate Magnets. ANDREAS GLATZ, Argonne National Laboratory, IGOR BELOBORODOV, Universidad de Chicago, VALERII VINOKUR, Argonne National Laboratory — I discuss the giant magnetoresistance (GMR) effect and its application to information storage technology. Iron-chromium multi-layer structures have been studied extensively, but there remain many questions in the field due to the complex behavior of the anti-ferromagnetic layer (Cr). Using our silicon micro-machined calorimeters, we examine the low temperature specific heat for a range of sputtered MML films grown under similar conditions to those used in industry. We have observed an enhanced electronic density of states in the Fe-Cr MMLs far beyond that of the iron or chromium individually. We compare this enhancement to the observed GMR behavior through a systematic study varying the thickness of the spacer layer.

9:00AM U32.00006 Influence of dipolar interactions on the formation of domains in layered Ni/Al2O3 nanocomposites. R. DAS, A. HEBARD, University of Florida, A. GUPTA, D. KUMAR, North Carolina Agricultural and Technical State University, S. OH, S. PENNYCOOK, Oak Ridge National Laboratory — Pulsed laser deposition has been used to fabricate Ni/Al2O3 multilayer composites in which Ni nanoparticles of uniform size in the range of 3-60 nm are embedded as layers in an insulating Al2O3 host. At fixed temperatures, the coercive fields show a well-defined critical size that delineates a crossover from single domain (SD) to multiple domain (MD) behavior. Most applications require that the particles be single domain with a uniform magnetization that remains stable with a sufficiently large anisotropy energy to overcome thermal fluctuations and beat the superparamagnetic limit, which establishes a temperature-dependent lower bound to the particle size (superparamagnetic limit). These considerations must take into account the effect of interactions on magnetic properties as is evident for high-density recording media where particles are very close to each other. The effect of dipolar interactions on the establishment of an upper bound to particle size ($d_c$), which defines the crossover from SD to MD behavior will be discussed. We show using coercivity measurements that, with increasing temperature, $d_c$ increases and then saturates due to attenuated dipolar interactions from thermally induced motions of neighboring randomly oriented particles.

9:12AM U32.00007 An investigation of quantum well states and magnetic properties of Co/Au/Ru(0001). J. CHOI, J. WU, Dept. of Physics, Univ. of California, Berkeley, CA 94720, F. EL GABALY, A.K. SCHMID, NCEM, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, Z.Q. QIU, Dept. of Physics, Univ. of California, Berkeley, CA 94720 — Quantum well state of Co/Au/Ru(0001) was investigated using Spin Polarized Low Energy Electron Microscopy (SPLEEM). Epitaxially grown Au on Ru(0001) at room temperature was annealed to $\sim$300 °C. Upon annealing, Au forms islands with atomically flat tops across stepped regions of Ru, forming local wedges of different Au thickness. Energy scans reveal clearly the existence of quantum well states in Au/Ru(0001). After depositing Co film on top of the Au, we found that the Curie temperature and the spin reorientation transition of Co film on the flat-top Au islands are different from that on the Au wetting layer. However the quantum well states of the Au layer have no effect on the Curie temperature and the spin reorientation transition of Co film.
9:24AM U32.00008 Angular Dependent Magnetic Susceptibility with Photoexcitation Studies on Prussian Blue Analog Thin Films¹, D.M. PAJEROWSKI, J.-H. PARK, M.W. MEISEL, Physics Department, University of Florida, F.A. FRYE, D.R. TALHAM, Chemistry Department, University of Florida — Prussian blue analog systems are the topic of ongoing research because of their novel physical effects. One such effect is persistent photoinduced magnetization, found in CoFe analogs. For such an optical system, in an attempt to maximize the material's interaction with incident photons, a thin film geometry is often utilized; this geometry can produce new effects [1]. Samples of different starting materials have been characterized with respect to photoinduced states, angular dependent susceptibility, film thickness, and chemical formula. Notably, magnetic anisotropies present in the systems show a dependence on the studied factors. One class of interesting starting materials are $\text{Rb}_2\text{Ni}_2[\text{Cr}(_3\text{Ni})_2]_3$, $\text{H}_2\text{O}$ and $\text{Rb}_2\text{Co}_2[\text{Fe}(_5\text{Co})_2]_3$, $\text{H}_2\text{O}$ heterostructures, generated by sequential adsorption on a Melinex substrate, that display behavior different than a noninteracting admixture of the two materials by themselves.

¹This work was supported, in part, by the National Science Foundation DMR-0305371 and DMR-0701400 (MWM) and NSF DMR-0543362 (DRT).

9:36AM U32.00009 Ferroelectric control of magnetism in BaTiO$_3$/Fe heterostructures¹, SARBESWAR SAHOO, University of Nebraska-Lincoln, SRINIVAS POLISETTY, CHUN GANG DUAN, SITARAM JASWAL, EVGENY TSYMBAL, CHRISTIAN BINEK — Multiferroics can offer the possibility to manipulate the cross coupled order parameters by conjugate electric and magnetic fields. Switching off ferroelectric order by an electric field for instance promises significant impact in the design of novel spintronics devices. Here we report on the reversible control of magnetism for a Fe thin film in proximity of a BaTiO$_3$ single-crystal. Large magnetization changes emerge in response to ferroelectric switching and structural transitions of BaTiO$_3$ controlled by applied electric fields and temperature, respectively. Interface strain coupling is the primary mechanism altering the induced magnetic anisotropy. As a result, coercivity changes up to 120% occur between the various structural states of BaTiO$_3$. Up to 20% coercivity change is achieved via electrical control at room temperature. Our all solid state ferroelectric-ferromagnetic heterostructures open viable possibilities for new technological applications.¹

¹Work supported by NSF through career DMR-0547887, the Nebraska Research Initiative (NRI), and by NSF MRSEC DMR-0213808.

9:48AM U32.00010 Griffiths phase and paramagnetism in ErCo$_2$³, FERNANDO BARTOLOME, LUIS M. GARCIA, ICMA, CSIC - Universidad de Zaragoza, JULIA HERRERO-ALBILLOS, Materiomics Science Dept., Cambridge University, ANTHONY T. YOUNG, Advanced Light Source, BLNL, TOBIAS FUNK, UCSF Physics Research Laboratory — A systematic study of the paramagnetic phase of ErCo$_2$ has recently allowed to identify the inversion of the net magnetization of the Co net moment with respect to the applied field well above the ferrimagnetic ordering temperature, $T_U$. This phenomenon, which we have denoted paramagnetism, may be related with the onset of a Griffiths-like phase in paramagnetic ErCo$_2$. We have measured SANS and ac susceptibility on ErCo$_2$ as a function of temperature, applied field, and excitation frequency. Several characteristics shared by systems showing a Griffiths phase are present in ErCo$_2$, namely the formation of ferromagnetic clusters in the disordered phase, the loss of analyticity of the magnetic susceptibility and its extreme sensitivity to an applied field. Our XMCD study of the Co magnetic moment flipping process show the occurrence of a pseudo-violation of the third Hund’s rule at the para- to paramagnetic “transition.”

³This research is supported by the Royal Society under a Wolfson Research Merit Award.

10:00AM U32.00011 Magnetostriiction close to the phase transition in Gd$_5$(Si$_2$Ge$_{1-x}$)$_2$Ge$_x$¹, R. L. HADIMANI, Y. MELIKHOV, J. E. SNYDER, D. C. JILES, Wolfson Centre for Magnetics, Cardiff University, CF24 3AA, U.K. — Gd$_5$(Si$_2$Ge$_{1-x}$)$_2$Ge$_x$ is a potential material for magnetic refrigeration. It has the highest magnetocaloric effect observed for the composition 0.41$\leq x \leq 0.5$ near its first order coupled magnetic-structural phase transition. We have investigated the relationship between the magnetic transition from ferromagnetic to paramagnetic phase and the structural transition from monoclinic to orthorhombic. A series of measurements have been carried out showing magnetostriective strain as a function of temperature at various magnetic field strengths and magnetostriction strain as a function of magnetic field at various temperatures with a magnetic field of up to 7 Tesla. There was fine structure observed in the magnetostriction curve at $H$ near the critical point. The magnetostriction measurements show that close to the critical temperature there is a sudden increase in the magnetostriction of about 100 ppm just before the field induced first order phase transition. This anomaly was observed for both strain vs. magnetic field at various temperatures and for strain vs. temperature at various magnetic field strengths measurements.

¹This work was supported, in part, by the National Science Foundation DMR-0305371 and DMR-0701400 (MWM) and NSF DMR-0543362 (DRT).

10:12AM U32.00012 Magnetostatic interaction between two thin nanotubes¹, EUGENIO E. VOGEL, Universidad de La Frontera, Temuco, Chile, OMAR SUÁREZ, PATRICIO VARGAS, Universidad Santa María, Valparaiso, Chile — We consider here the magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary magnetic interaction between two identical tubes, characterized by: total magnetization $M$, length $2L$, external radius $R_e$, internal radius $R_i$. Following most of the experimental realizations we consider very thin tubes, namely, $(R_e-R_i) \ll 2L$, analytic integration over the interaction of elements on each tube, and numeric integration for general cases. These results are compared with two independent results: a) the tubes are far apart so they can be considered solid nanowires: b) each tube is considered as a set of elementary

¹Fondecyt 1060317

10:24AM U32.00013 Kondo-like features in chemically pure magnetic atomic-size contacts, M. REYES-CALVO, JOAQUIN FERNANDEZ-ROSSERT, CARLOS UNTIATED, LT-Nonlab. Depto. de Física Aplicada, Universidad de Alicante — The influence of magnetic frustration in the electronic transport in atomic sized contacts is not yet clear. However, certain features systematically appear in the conductance measurements of magnetic atomic contacts. Specifically, the spectroscopy of atomic size contacts of Ni, Fe or Co reveal the existence of a characteristic significant peak or dip at zero bias that is not present in the case of non-magnetic materials. We have measured the differential conductance as a function of bias at 4K on two hundred monatomic contacts of Ni, Fe and Co fabricated by STM. The zero bias anomaly has been analyzed as using the Kondo- Fano lineshape typical of magnetic adatoms in non-magnetic surfaces. The statistical analysis of the data results in Kondo temperatures around 250 K, 120 K and 80 K for Ni, Co and Fe respectively. A Kondo-like behaviour could arise in chemically pure magnetic contacts if tip atoms behave different due to their smaller coordination.

10:36AM U32.00014 ABSTRACT HAS BEEN MOVED TO SESSION K1
The nitrogen vacancy releases electrons in the system which changes the Mn magnetic interactions in GaN in the presence of nitrogen and gallium vacancies. Previous studies have found the nitrogen vacancy has the lowest formation temperature $T_c$ conductors from first principles.


Thus, both the nitrogen and gallium vacancy are found to impede ferromagnetism. This work is supported by AFOSR-FA 9550-05-1-0462.

3 Supported by NSF-ECCS CAREER and US ONR.

8:36AM U33.00002 Effect of vacancies on ferromagnetism in GaN:Mn dilute magnetic semiconductors from first principles1, PAUL LARSON, SASHI SATPATHY, University of Missouri — In spite of considerable interest in ferromagnetism of the dilute magnetic semiconductor GaN:Mn, the nature of ferromagnetism is still quite controversial. Experimental values for the Curie temperature $T_c$ vary widely depending upon the details of the impurity concentrations. We have performed ab initio density functional studies of the magnetic interactions in GaN in the presence of nitrogen and gallium vacancies. Previous studies have found the nitrogen vacancy has the lowest formation energy. The nitrogen vacancy releases electrons in the system which changes the Mn d$^5$ state to a half-filled Mn d$^4$ state, so that the antiferromagnetic superexchange becomes dominant. The naive picture of Ga vacancies is the release of holes into the system which should increase ferromagnetism. However, we find an antiferromagnetic interaction for the Ga vacancy, as well in agreement with Mahadevan’s work1. This can be attributed to the localized nature of the holes states which do not participate in the transport. This hole localization from the Ga vacancy has been demonstrated using the virtual crystal approximation.

Thus, both the nitrogen and gallium vacancy are found to impede ferromagnetism. This work is supported by AFOSR-FA 9550-05-1-0462.


8:48AM U33.00003 Effect of magnetic short-range order on spin disorder resistivity. ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA, MARK VAN SCHILFGAARDE, Department of Chemical and Materials Engineering, Arizona State University, Tempe, Arizona, USA, JULIAN VELEV, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA — Spin-disorder resistivity (SDR) of Fe and Ni is studied using the noncollinear density functional theory. The Landauer conductance is averaged over random disorder configurations and fitted to Ohm’s law. In the fully disordered state, SDR for Fe close to $T_c$ is 2 orders of magnitude smaller than the experimental value by a factor of 2.3. This indicates either strong magnetic short-range order (MSRO) or reduced local moment above $T_c$ for Ni. The temperature dependence of SDR for Fe was studied using the mean-field approximation and the Monte Carlo method applied to the classical nearest-neighbor Heisenberg model. Both methods gives the same magnetization dependence of SDR that is in excellent agreement with the results for the isotropic s-d model. Further using the Reverse Monte Carlo method we generated disordered spin structures with strong MSRO. We found the resulting SDR is not significantly different than for Monte Carlo and mean-field methods. This result indicates that for Fe MSRO is not very important for SDR.

9:00AM U33.00004 First-Principle theory of Longitudinal Spin-Fluctuations at high temperatures for itinerant ferromagnets. SERGII KHMELEVSKYI, Center for Computational Material Science, Vienna University of Technology, ANDREI V. VONsovsky, Department of Materials Physics, Royal Institute of Technology, Stockholm, Sweden, PETER MOHN, Center for Computational Material Science, Vienna University of Technology, BJORNE JOHANSSON, Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden — We have developed a framework for calculating parameters of effective magnetic Hamiltonian, which includes transverse as well as longitudinal spin fluctuations (LSF) on equal footing. The method is based on the set of constrained calculations within a Local Spin-Density Approximation and Coherent Potential Approximations. The used effective Hamiltonian is similar to those derived in Moriya-Takahashi theory approximating between local and weak itinerant limits of magnetism. The Curie temperature, magnetic susceptibilities and field induced magnetizations were calculated both for Fe and Ni in good agreement with experiment. The importance of LSF contribution even for qualitatively correct description of magnetism of Ni is demonstrated. The first principles criteria for magnetic moment ‘itineracy’, based on fixed spin moment constrained calculations of a magnetic impurity in the Disordered Local Moment host, is established and applied to various magnetic systems. In particular, the famous Rhodes-Wohlfarth plot has been revisited. It is found that in some cases, like VAu$_2$, the magnetic moments have very local character in contrast to their long-standing interpretation as weak itinerant ferromagnets.
9:12AM U33.00005 Calculation of diamagnetic susceptibility in Cu, graphite and Bi from band-structure1, G. SAMOYLUK, J. SCHMALIAN, B. HARMON, S. BUD’KO, P. CANFIELD, AmesLab/Dept. of Physics, ISU — Since early pioneering work on the orbital diamagnetism of free electrons[1] the problem of calculation of diamagnetic susceptibility has attracted attention in systems such as graphite and bismuth. Recent interest in this problem has been motivated by the unconventional electronic properties of mono- and multilayered graphenes. These materials demonstrate large orbital diamagnetism caused by a specific type of band dispersion: a crossing of two bands, each with linear dispersion near the Fermi level. Significant progress in the theoretical description of orbital diamagnetism of electrons in periodic potentials was achieved by Fukuyama[2], with an exact expression for diamagnetic susceptibility, but with an approximation for band dispersion put in by hand. As an alternate approach, we use band structure obtained from a first-principles calculation (LMTO). The orbital susceptibility was calculated for Cu, as an example of a metal with small orbital diamagnetism, as well as for graphite and Bi, materials with known, large diamagnetic susceptibilities. [1] L. Landau, Z. Physik. 64, (1930) 629. [2] H. Fukuyama, Prog. Theor. Phys. 45, (1971) 704.

1Supported by the DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

9:24AM U33.00006 Magnetic Moment of MnSi1, ROBERT COLLYER, DANA BROWNE, Louisiana State University — MnSi is a metallic helimagnet below 29 K. Density functional theory predicts that it has a moment of 1.0 $\mu_B$/Mn, which is much larger than the measured value of 0.4 $\mu_B$/Mn. By adding a Hubbard-U correction, we have found a ground state with a moment consistent with the experimental value. These solutions possess a novel quadrupolar spin ordering. We discuss their behavior under pressure and in a magnetic field.

9:36AM U33.00007 ABSTRACT WITHDRAWN

9:48AM U33.00008 Piezomagnetic effect in Mn-based antiperovskites, RENAT SABIRIANOV, PAVEL LUKASHCHEV, University of Nebraska, Omaha, KIRILL BËLASHCHENKO, University of Nebraska, Lincoln — We predict large piezomagnetic effect in Mn-based antiperovskites. The magnetic ground state is determined to be the non-collinear $5g$ structure, which can be viewed as a sequence of alternating layers of clockwise and counterclockwise triangular spin currents in (111) plane, resulting in the zero total magnetization of the system. We use PAW method (VASP) within PBE generalized gradient approximation. We find that the system develops non-zero magnetization under biaxial strain due to the lowering of the crystal symmetry from cubic to tetragonal. The system exhibits linear magnetization dependence on the applied strain over the moderate range (up to 1%) of the latter. The magnetization under strain appears as a result of the rotation of local magnetic moments (LMM) on Mn atoms in Mn$_2$N$_2$ plane. Besides, the system exhibits biaxial anisotropy under strain. We propose using the observed piezomagnetic effect to build the magnetoelectric perovskite ferroelectric – antiperovskite piezomagnetic heterostructures. The estimated magnetoelectric coefficient is $\sim 2*10^{-9}$s/m. Because of the piezomagnetic effect, Mn-based antiperovskites can be used in memory cells with electric control of magnetization. It can also be applicable in spintronics, as the system develops a net polarization of up to 30% under external strain.

10:00AM U33.00009 Spin Flip in the Presence of a Complex Absorbing Potential, FRANK MARSIGLIO, FATHI DOGAN, CINDY BLOIS, WONKEE KIM, University of Alberta — We examine the impact of a complex absorbing potential on electron transport, both in the continuum and on a lattice. This requires the use of non-Hermitian Hamiltonians; the required formalism is briefly outlined. The lattice formulation allows us to study the interesting problem of an electron interacting with a stationary spin, and the subsequent time evolution of the electron and spin properties as the electron is absorbed after the initial interaction. Remarkably, the properties of the localized spin are affected ‘at-a-distance’ by the interaction of the (now entangled) electron with a complex potential.

10:12AM U33.00010 Giant Zeeman electric-dipole resonance in antiferromagnetic conductors, REVAZ RAMAZASHVILI, LPTMS, Orsay — Essential dependence of the electron g-factor on the quasiparticle momentum is a fundamental and, so far, largely overlooked property of antiferromagnetic conductors. It leads to a number of remarkable phenomena, such as excitation of spin flip transitions by AC electric field. Absorption intensity of these transitions exceeds that of the Electron Spin Resonance by some four orders of magnitude. I develop a theory of this phenomenon in a weakly doped antiferromagnetic insulator. The predictions may be relevant for a number of antiferromagnetic conductors, ranging from chromium to electron-and hole-doped cuprates, to organic conductors with spin density wave, and to heavy fermion antiferromagnetic metals.

10:24AM U33.00011 Electronic properties and magnetic moments of Mn$_x$Si$_{1-x}$ for $x < 5%$. MICHAEAL SHAUGHNESSY, RYAN SNOW, CHING YAO FONG, University of California Davis Physics Department — Recently, there have been experimental reports about Mn$_x$Si$_{1-x}$ alloys. All show great promise for room temperature spintronic applications. We report on theoretical studies of the electronic properties of Mn$_x$Si$_{1-x}$ for $x < 5\%$, using first principles density functional methods. For the Mn-doped Si, we consider three configurations of the Mn impurities: nearest neighbor (nn), second nearest neighbor (snn), and a three-atom chain configuration. For the nn and snn configurations, the ferromagnetic and antiferromagnetic phases have been compared. The magnetic moment/unit-cell for the nn and ferromagnetic configurations is smaller than for the ferromagnetic snn and chain configurations. The reason will be given. Supported in part by NSF grant: ESC-0725902.

10:36AM U33.00012 Monte Carlo simulation of giant magnetoresistance1, GASTON BARBERIS, IFGW - Unicamp, 13083-970 Campinas, SP, Brazil — Monte Carlo method was used to simulate giant magnetoresistance in solids. A square lattice, composed by Ising spins, was generated by the usual Monte Carlo method, with periodic conditions for the borders. Resistivity was measured considering the number of clusters connected between right and left sides of the lattice, with and without applied magnetic field. The calculation of the number and surface of the connecting clusters was calculated using the Hoshen-Kopelman algorithm [1]. As we developed previously pseudorandom non-periodic numbers [2], which allows that the sizes of the clusters as big as necessary, and the steps near the transition as small as desired. This allowed a detailed study near the percolation region, over and below the magnetic transition. Three dimensional lattices, and models other than Ising for the spin coupling are natural extension of the calculation. [1] J. Hoshen and R. Kopelman, Phys. Rev. B14, 3438 (1976) [2]G.E. Barbaris, Physica B 398, 468 (2007)

1The author acknowledge financial help from FAPESP, Brazil

10:48AM U33.00013 Propagators for Hamiltonians with Spin-Orbit Coupling, BAILEY HSU, JEAN-FRANCOIS VAN HUELE, Brigham Young University — Quantum mechanical propagators can be used to understand the dynamics of electrons in confined electromagnetic environments. We extend the propagator formalism to include the spin degree of freedom for spin-orbit coupling potentials in two-dimensional geometries. The 2x2 spin propagator allows us to follow the evolution in time and space of the spin-components of localized wave packets. We apply the technique to Rashba and Dresselhaus interactions and present graphical displays of the corresponding spin motions.
8:12AM U35.00002 Determination of best models for adsorption of hydrogen in boron-doped carbon nanoparticles¹, RAINA CEPEL, MATTHEW BECKER, CARLOS WEXLER, PETER PFEIFER, University of Missouri — Nanoporous carbon offers significant hydrogen storage capacities at low pressures in reversible conditions. Storage is achieved by physical adsorption of molecular hydrogen (H₂) on the surface of nanometer-size pores in the carbon matrix. Within the ALL-CRAFT collaboration (http://all-craft.missouri.edu), we conduct a proof-of-concept study of the prediction that boron-doped nanoporous carbon can store as much as 8 weight% at 47 bar and room temperature. By comparing theoretical and experimental H₂ adsorption isotherms for intrinsic and doped carbon, we determine which adsorption models and scenarios (e.g. localized vs. mobile) are consistent with experimental evidence.

¹University of Missouri Research Board (RB-06-040), U.S. Department of Defense (N00164-07-P-1306), U.S. Department of Energy (DE-FG02-07ER46411)

8:24AM U35.00003 Metal clustering and catalytic spillover on the nanotubes and graphene for hydrogen storage, FENG DING, PAVEL KRASNOV, YU LIN, BORIS I. YAKOBSON, Rice University — Energies and kinetic barriers associated with transition metal (Sc) clustering on a single-walled carbon nanotube (SWNT) and graphene were studied by all-electron density functional method. The analysis shows that the binding energy of Sc atom on SWNT is highly sensitive to the tube diameter and chirality. The metal atoms do cluster on common SWNT, with diameters ~1-2 nm. Hydrogen binds to the metal cluster chemically and thus opens a way for hydrogen storage via catalytic spillover. However, the hydrogen chemisorption on graphene receptor-substrate is difficult to reconcile with a single H atom binding to carbon being weaker than it is within initial molecular H₂. This paradox is resolved by presenting the process as phase nucleation. Atomistic calculations bridge remarkably with the macroscopic-continuum description, and show a feasible path to 7.7 wt% H-content at nearly ambient conditions. P. O. Krasnov, F. Ding, et al., J. Phys. Chem. C, in press (2007).

8:36AM U35.00004 Hydrogen Storage in Ti Doped Nano Porous Graphene¹, SA LI, PURU JENA, Virginia Commonwealth University, DEPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — Clustering of Ti on carbon nanostructures has proved to be an obstacle in their use as hydrogen storage materials. Using density functional theory we show that Ti atoms will not cluster when doped into nanoporous graphene. With each Ti atom binding up to four hydrogen molecules with an average binding energy of 0.54 eV/H₂, this material can be ideal for storing hydrogen. Equally important, nanoporous graphene is magnetic with or without Ti doping, but magnetism disappears when fully saturated with hydrogen. This novel feature suggests that nanoporous graphene can also be used as a hydrogen sensor.

¹This work is supported in part by a grant from the Department of Energy. We would like to thank the PNNL for computer support.

8:48AM U35.00005 Graphenic C₃N₄: A New Template for Metal Decoration and Hydrogen Adsorption¹, YI ZHANG, University of Nevada, Las Vegas, HONG SUN, Shanghai Jiao Tong University, China, CHANGFENG CHEN, University of Nevada, Las Vegas — From density functional theory calculations we identify a graphenic C₃N₄ (g-C₃N₄) structure as an excellent template for stable and well dispersed decoration of alkali and transition metals which, in turn, exhibits a high capacity for hydrogen adsorption with binding energies (a few tenths of eV) suitable for mobile applications. The unique porous micro-structural sites of g-C₃N₄ accommodate the excess N lone-pair electrons and promote strong hybridization between the orbitals of N and metal atoms. It plays a key role in overcoming the tendency of metal-atom clustering that has plagued other proposed hydrogen storage media. These metal decorated g-C₃N₄ may also prove useful in a variety of catalytic and sensing applications.

¹This work was supported by the DOE Coopera-tive Agreement DE-FG36-05GO85028 and DE-FC52-06NA26274 at UNLV and by the NSF grants No.10574089 and No. 50532020 at SJTU.

9:00AM U35.00006 Hydrogen Storage in Titanium-decorated Boron Buckyball, JIA LI, GANG ZHOU, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing 100084, PR China, HOONKYUNG LEE, JISOOK IHH, Department of Physics and Astronomy, Seoul 151-747, Korea — Using first-principles electronic structure calculations, we investigate the potential of Ti-decorated B₈₀ for hydrogen storage medium. The Ti-decorated B₈₀ has the merit of an unexpected large binding energy of a Ti atom to B₈₀ which can overcome the problem of metal clustering. Up to four hydrogen molecules are found to be adsorbed on a single Ti atom coated on B₈₀. At high Ti coverage, we show that the Ti-decorated B₈₀ adsorbs up to 5 wt% hydrogen and the calculated binding energy falls in the desirable range of 0.2-0.6eV/H₂ which is suitable for reversible hydrogen storage at room temperature, near-ambient-pressure conditions.

9:12AM U35.00007 Sequential Dissociative Chemisorption of H₂ on Ti₃H Cluster¹, T.J. DHLIP KUMAR, P. TARAKESHWAR, N. BALAKRISHNAN, Department of Chemistry, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89154 USA — Ti nanoparticles have received much attention due to their superior catalytic properties in potential hydrogen storage materials for fuel cell applications. In this study, we show that the energetically stable distorted icosahedral Ti₃H cluster has excellent H₂ adsorption and desorption properties and lead to stable structures upon hydrogen cycling. H₂ adsorption initially leads to a highly stable Ti₃H₂₀ cluster and on further saturation yields the Ti₄H₅ cluster. The chemisorbed H atom in Ti₃H₂₀ occupies above the face of the triangular planes of Ti₁₂ whereas in Ti₁₂H₂₀, H atoms remain dangling above the apex Ti edges. The three coordinated H in Ti₄H₂₀ has higher chemisorption and desorption energies than the fully saturated Ti₁₂H₂₀ cluster. This type of multi-center H-bonds with varied chemisorption energies is structurally significant since adsorption and desorption rate processes could be controlled and deserve attention as potential candidates for hydrogen storage materials.

¹This work is supported by DOE Grant DE-FG36-05GO85028.
Cocaine detection using piezoresistive microcantilevers

— A Precursor to Hydrogen Storage

1 Work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

Department of Physics, University of Tennessee — Sensitive and inexpensive sensors play a significant role in the analysis of drugs and drug metabolites. Specifically, reliable in vivo detection of cocaine and cocaine metabolites serves as a useful tool in research of the body’s reaction to the drug and in the treatment of the drug addiction. We present here a promising cocaine biosensor to be used in the human body. The sensor’s active element consists of piezoresistive microcantilevers coated with an oligonucleotide-based aptamer as the cocaine binder. In vitro cocaine detection was carried out by flowing a cocaine solution over the microcantilevers. Advantages of this device are its low power consumption, its high sensitivity, and its potential for miniaturization. Current studies indicate that silicon carbide nanotubes coated with an oligonucleotide-based aptamer as the cocaine binder. In vivo cocaine detection was carried out by flowing a cocaine solution over the microcantilevers. Advantages of this device are its low power consumption, its high sensitivity, and its potential for miniaturization.

8:00AM U36.00001 Cocaine detection using piezoresistive microcantilevers

1, BERNADETA SRJANTO, Department of Electrical Engineering, University of Tennessee, CHRISTINE F. CHENEY, DAVID L. HEDDEN, ANTHONY GEHL, THOMAS L. FERRELL, Department of Physics, University of Tennessee — Sensitive and inexpensive sensors play a significant role in the analysis of drugs and drug metabolites. Specifically, reliable in vivo detection of cocaine and cocaine metabolites serves as a useful tool in research of the body’s reaction to the drug and in the treatment of the drug addiction. We present here a promising cocaine biosensor to be used in the human body. The sensor’s active element consists of piezoresistive microcantilevers coated with an oligonucleotide-based aptamer as the cocaine binder. In vitro cocaine detection was carried out by flowing a cocaine solution over the microcantilevers. Advantages of this device are its low power consumption, its high sensitivity, and its potential for miniaturization.

1 This research was supported by the National Institute on Alcohol Abuse and Alcoholism NIAAA under Contract No. N01AA23012.

8:00AM U36.00002 Bioinspired optical sensing of picomolar concentrations of lead in solution.

1, ANUSHREE SAHA, VLADISLAV YAKOULEV, University of Wisconsin-Milwaukee, UNIVERSITY OF WISCONSIN-MILWAUKEE TEAM — Lead poisoning is a life threatening medical condition, which can cause irreversible neurological, cardiovascular and reproductive damage. Despite of an extensive research, the minimum amount of lead to be considered hazardous is not yet known. The biophysical interactions of minute quantities of lead with blood are also poorly understood. Albumin being the most important binder and transporter in blood, is known to interact with lead ions in solution. In this report, we present the first experimental evidence that picomolar concentrations of lead strongly affect albumin properties in solution. High precision difference Raman and excitation-emission fluorescence spectroscopies are employed to identify the effect of lead ions on albumin. Both spectroscopies proved to be very effective in detecting lead poisoning at a very early stage, setting a new course for bio-inspired inexpensive platform of lead sensing.

1 University of Wisconsin-Milwaukee

8:24AM U36.00003 Nanofluidic redox-cycling in electrochemical biosensing applications

, BERNARD DE WOLFRUM, MARCEL ZEVENBERGEN, SERGE LEMAY, Kavli Institute of Nanoscience, Delft University of Technology — We have developed a chip-based nanofluidic device which amplifies the sensitivity in electrochemical biosensing applications by orders of magnitude. The amplification is based on rapid redox-cycling between plane parallel electrodes inside a nanochannel. We show that it is possible to monitor the signal of less than one hundred molecules residing in the active area of the nanofluidic sensor. The small number of molecules is reflected in the noise spectrum of the device. In particular, we obtain high sensitivities when detecting catecholamines, which comprise an important group of hormones and neurotransmitters such as serotonin and dopamine. Furthermore, due to the nanochannel design, the sensor is immune to interference by molecules undergoing irreversible redox reactions. We demonstrate the selectivity of the device by detecting target molecules in the presence of ascorbic acid whose oxidized form is only stable on the order of milliseconds. The interference of ascorbic acid is usually a challenge in the detection of catecholamines in biological samples.

8:36AM U36.00004 Detection of Target Biomolecules by Magnetic Reporting Using Rod-Like Nanosensors

, R.P. GUERTIN, E. GOLDBERG, T.P. HARRAH, S. SONKUSALE, K. PARK, Tufts University, S. SUN, Brown University, J. I. OH, M. NAUGHTON, Boston College — We describe the ongoing development of a device to assay a variety of cellular, viral and molecular targets by measuring the increase of the Brownian relaxation time, τ in solution of magnetically-tagged nanoscale detectors. The shift shows as a frequency reduction of the peak of the complex magnetic susceptibility, χ(ω)^−1. Measurements of χ(ω) with 12 nm monodisperse nanoparticles of CoFe2O4 coated with polyethylene glycol reveal spectra with the narrowest lines yet reported. Thin avidin coating of these particles reveals small shifts in χ(ω)^−1. Bacteriophage T4 tail fibers, engineered to specific lengths (30-150 nm), were employed as the platform for magnetic nanoparticle attachment and at the other end for an inserted target peptide epitope. Attachment of the nanoparticles to bacteriophage T4 tail fibers was successful, though no detectable shifts in χ(ω)^−1 were detected due to weak attachment. The advantages associated with non-spherical geometry detectors will be discussed, as well preliminary measurements with rare earth oxide magnetic nanoparticles. Progress on miniaturization and low power requirements of the electronic detection system will be reported. Supported by NERC/BEID (NIAID).

8:48AM U36.00005 A Ringdown Breath Analyzer for Diabetes Monitoring: Breath Acetone in Diabetic Patients

, CHUJII WANG, Dept. of Phys, and the ICET, Mississippi State University, Starkville, MS 39759, cw175@msstate.edu, ARMSTRONG MBI, Dept. of Phys, and the ICET, Mississippi State University, Starkville, MS 39759, MARK SHEPHERD, Endocrinology Consultants Center, 670 Crossover Rd. Tupelo, MS, 38801 — It is highly desirable for millions of diabetic patients to have a non-blood, non-invasive, point-of-care device for monitoring daily blood glucose (BG) levels and the adequacy of diabetic treatment and control. Cavity ringdown spectroscopy, due to its unique capability of high sensitivity, fast-response, and relatively low cost for instrumentation, has the potential for medical application through non-invasive analysis of breath biomarkers. We report the first ringdown acetone breath analyzer for clinic testing with diabetic outpatients. The instrument was set in a clinic center and 34 outpatients (24 T1D and 10 T2D) were tested during a four-day period. 10 T1D subjects and 15 non diabetic persons were tested in our laboratory. Three juvenile-onset T1D subjects were selected for a 24-hr monitoring on the variations of breath acetone and simultaneous BG level. In this talk, we present our research findings including the correlations of breath acetone with BG level and A1C.
9:00AM U36.00006 Integrating Different Types of Nanowire Sensors in a Large Array1, Yaping DAN, University of Pennsylvania, STEPHANE EVOY, University of Alberta, A.T. CHARLIE JOHNSON, University of Pennsylvania — Biological olfactory systems have a key structural feature: different types of sensors in a large array. Humans, for example, possess several hundred distinct types of sensing cells, a level of sensor diversity not yet achieved in artificial olfactory systems. Here, we demonstrate a simple and low-cost electrochemical approach to integrate large numbers of different types of nanowire sensors in an array on the same silicon wafer. In our approach, nanowires are grown inside an on-chip nanochannel template by electrochemistry with each horizontal channel connected to a gold electrode. This design allows for addressable synthesis of a specific type of nanowire in specified channels by providing a voltage to the electrodes connecting to those channels. The process can be further repeated to produce different types of nanowires in other channels using different electroplating solutions. The scale and diversity of this array have a potential to compete with those of biological olfactory systems and the synthesis process is cost-effective enough for commercialization.

1This work was supported by the National Science Foundation NIRT Grant #0303981 and ARO Grant.

9:12AM U36.00007 Compact Femtosecond-Millisecond Transient Absorption Spectrometer, ELIZABETH CARROLL, MELISSA HILL, DORTE MADSEN, KONSTANTIN MALLEY, DELMAR LARSEN, Department of Chemistry, University of California — The measurement of population dynamics in biological, chemical, and solid-state samples occurring over 10−13-10−1 seconds requires a combination of transient absorption techniques, typically involving different laser systems and detection electronics (e.g., femtosecond transient absorption and nanosecond flash photolysis). The difficulty in exactly matching excitation conditions often prohibits connecting ultrafast and longer time measurements, particularly in samples exhibiting nonlinear kinetics. We present a simple solution to bridge the femtosecond and microsecond domains with an inexpensive modification of a kHz amplified Ti:Sapphire laser. By introducing a secondary pulse-picker between the laser oscillator (75 MHz) and amplifier, we can electronically delay unamplified 800-nm probe pulses in 13.3-ns steps. The 5-nJ pulses seed a photonic crystal fiber to produce a supercontinuum (450-1100 nm) for broadband probing. We demonstrate the system capability by resolving formation and decay dynamics, spanning 10 decades (10−14-10−1 s), of photoexcited solvated electrons in sinapic acid, and triplet states and quinonoid intermediates in Vitamin B6.

9:24AM U36.00008 Realization of Confocal and Hyperspectral Microscopy via Compressive Sensing, TING SUN, Rice University, DHARMPAL TAKHAR, JASON LASKA, MARCO DURARTE, VIVEK BANSAL, RICHARD BARANIUK, KEVIN KELLY — Given its important role, factors such as sensitivity, resolution, dwell time, and bandwidth limit are critical parameters for detectors in modern microscopy. A new method known as compressive sensing has emerged, which greatly improves the imaging resolution of these detectors. In our configuration, a digital micromirror device randomly but controllably modulates the light before it is collected at the detector. This process simultaneously compresses the signal because the measurement projects the signal onto a white-noise basis. Subsequently, the data from this incoherent basis is reconstructed into a complete real-space image. Given its compressive nature, far fewer measurements are required than the total number of pixels which greatly decreases the acquisition time of the signal. In addition, the intensity of the compressed signal at the detector is much greater than its raster scan counterpart and therefore results in greater signal sensitivity and improved image quality. These advantages make compressive sensing particularly attractive for use in hyperspectral and confocal microscopy.

9:36AM U36.00009 Fabrication of robust superconducting granular aluminum/palladium bilayer microbolometers with sub-nanosecond response1, THOMAS WILSON, Marshall University — We provide a convenient recipe for fabricating reliable superconducting microbolometers as acoustic phonon detectors with sub-nanosecond response, using image-reversal optical lithography and dc-magnetron sputtering, and our recipe requires no chemical or plasma etching. Our approach solves the traditional problem for granular aluminum bolometers of unreliable (i.e., non-Ohmic) electrical contacts by sequentially sputtering the granular aluminum film and then a palladium capping layer. We use dc calibration data, the method of Danilchenko et al., and direct nanosecond-pulsed photoexcitation to obtain the microbolometer’s characteristic current, thermal conductance, characteristic relaxation time, and heat capacity. We also demonstrate the use of the deconvolution algorithm of Edwards et al., to obtain the phonon flux in a heat pulse experiment with nanosecond resolution.

1Support provided by NSF ECCS 062060.

9:48AM U36.00010 Highly Sensitive Photodetector Based on a Self-assembled Organic Single Submicrometer Ribbon, JIAN WANG, YAN ZHOU, LEI WANG, South China University of Technology, JIAN PEI, Peking University — We demonstrated a highly sensitive air-stable photodetector based on a single submicrometer organic crystalline ribbon self-assembled from a condensed benzo thiophene via solution process. The low cost and simple solution process was employed in the device fabrication process from the submicrometer ribbons preparation to the deposition on the substrate. The photodetector gain is up to 1.3 × 10^3, while the responsivity is about 420 A/W at the field of 2 × 10^5 V/cm. The highest on/off ratio reaches around 1000. The performance is comparable to that of photodetectors based on inorganic nanowires, and even better than those based on carbon nanotube or other bilayer molecular self-assembled nanotubes. In addition, the photo-switching properties to those organic photodetectors were investigated with different metal electrodes. The results show that the surface states created by the thermal evaporation of the heavy gold atoms are responsible for the high photo gain and the slow photocurrent decay. To our best knowledge, this is the first report on photodetectors based on crystalline organic 1D submicrometer ribbons self-assembled via solution process, which combine both advantages of intrinsic properties of the 1D crystalline structure and the simplicity of the solution process.

10:00AM U36.00011 Single carbon nanotube syringe: A model for the study of liquid transport through individual carbon nanotubes, GUANGYU CHAI, Apollo Technologies, Inc. 205 Waymont Court #111, Lake Mary, FL 32746, USA, LEE CHOW, Department of Physics, University of Central Florida, Orlando, FL 32816-2385, USA — The hollow structure of the carbon nanotubes (CNT) and their ability to translocate through plasma membrane of a living cell provide a significant chance to use them as a nano syringe for the delivery of therapeutically active molecules into a live cell. However, the size and the extremely high aspect ratio of the CNTs make the nano syringe device difficult to realize. We successfully prepared a monolithic multwall CNT with a graphitic shield by chemical vapor deposition technique. The graphitic shield provides a handle which allows the manipulation of the supported CNTs. A single CNT syringe device is fabricated with focused ion beam technique. The well-controlled liquid transport through individual CNT is demonstrated.
8:00AM U37.00001 Resistance oscillations in two-dimensional electron systems due to resonant acoustic phonon scattering\(^1\), MICHAEL ZUDOV, ANTHONY HATKE, WENHAO ZHANG, University of Minnesota, LOREN PFEIFFER, KEN WEST, Bell Labs, Alcatel-Lucent — A few years ago a new class of resistance oscillations was discovered in two-dimensional electron systems subject to weak magnetic fields and elevated temperatures [1]. It was proposed that oscillations originate from resonant interaction with acoustic phonons made possible by virtue of a special selection rule which favors electron backscattering. In contrast to other types of magneto-resistance oscillations, such as those appearing under application of microwave or dc electric fields, phonon-induced resistance oscillations (PIRO) have not received much attention and remain poorly understood. Of particular interest are the period and the phase of PIRO, relative contribution and nature of different phonon modes, and the effect of temperature and sample parameters. This talk will briefly review prior and new experimental results and discuss open issues.


\(^1\)This work is supported by NSF DMR-0548014.

8:12AM U37.00002 Effect of dc electric field on resonant acoustic phonon scattering in two-dimensional electron systems\(^1\), WENHAO ZHANG, MICHAEL ZUDOV, University of Minnesota, LOREN PFEIFFER, KEN WEST, Bell Labs, Alcatel-Lucent — We study [1] the effect of dc electric field on transport properties of two-dimensional electron systems in which resonant acoustic phonon scattering dominates linear response resistivity. We observe that dc electric field strongly modifies phonon resonances, transforming resistance maxima into minima and back into maxima. Further, phonon resonances are enhanced dramatically in the non-linear dc response and can be detected even at low temperatures. Most of our observations can be explained by dc-induced (de)tuning of the acoustic phonon resonances and intra-Landau level impurity scattering. We also observe a dc-induced zero-differential resistance state and a resistance maximum which occurs when the electron drift velocity approaches the speed of sound.


\(^1\)This work is supported by NSF DMR-0548014.

8:24AM U37.00003 Effect of electron-phonon scattering on magneto-transport in 2DES, M. G. VAVILOV, University of Wisconsin — We evaluate the contribution of electron-phonon scattering to the non-linear magneto-resistance of two-dimensional electron systems (2DES). Both linear [1] and differential [2] magneto-resistances show oscillatory dependence on the applied magnetic field in high mobility 2DES. These oscillations originate from the relation between the change of electron energy in a scattering event and the cyclotron frequency. In case of electron scattering with phonons in dc electric fields, the change in electron energy is equal to the sum of the energy of an emitted or absorbed phonon and the change of the electrostatic electron energy due to the shift of an electron cyclotron trajectory. We show that the electrostatic contribution in sufficiently strong fields moves the position of maxima and minima of the differential magnetoresistance. We also explain why the phonon-induced magneto-oscillations exist in the linear response regime only at moderately high temperatures, but appear at significantly lower temperatures in stronger electric fields. [1] M.A. Zudov, et al., Phys. Rev. Lett. 86, 3614 (2001). [2] W. Zhang, et al., arXiv:0711.1547v1 (2007).

8:36AM U37.00004 Non-linear dc response in microwave-irradiated two-dimensional electron systems: interplay between ac and dc induced effects\(^1\), ANTHONY HATKE, WENHAO ZHANG, MICHAEL ZUDOV, University of Minnesota, LOREN PFEIFFER, KEN WEST, Bell Labs, Alcatel-Lucent — We study nonlinear dc response of a high-mobility two-dimensional electron system subject to microwave (ac) excitation and weak magnetic fields. Recent experiments [1] studied resistance at different dc excitations as a function of the ratio of the microwave frequency to the cyclotron frequency, \(\epsilon \omega_c\). Here, we examine oscillations in microwave photoconductivity as a function of dc excitation, at different values of \(\epsilon \omega_c\). We find that, for the most part, the oscillation period is the same as in the dark resistivity, and the phase is determined by microwave-induced oscillations at zero dc bias, consistent with the earlier results. However, at some excitation values previously associated with resistance maxima, this approach revealed resistance minima indicating saddle points in the resistivity. We further observed that the oscillation amplitude itself oscillates as a function of \(\epsilon \omega_c\), with the oscillations strongly suppressed near half-integral values. These findings indicate the limitations of the simplified resonant condition proposed in Ref. 1, and might stimulate further theoretical studies.


\(^1\)This work is supported by NSF DMR-0548014.

8:48AM U37.00005 Zero differential resistance state in 2D dimensional electron system in strong magnetic field\(^1\), SERGEY VITKALOV, JING-QIAO ZHANG, The City College of New York, A. A. BYKOV, A. K. KALAGIN, A. K. BAKAROV, Institute of Semiconductor Physics, 630090 Novosibirsk, Russia — We report the observation of a zero differential resistance state (ZDRS) in response to direct current above a threshold value \(I > I_d\), applied to a two-dimensional system of electrons at low temperatures in a strong magnetic field. Entry into the ZDRS, which is not observable above several Kelvins, is accompanied by a sharp dip in the differential resistance. Additional analysis reveals instability of the electrons for \(I > I_d\) and an inhomogeneous, non-stationary pattern of the electric current. We suggest that the dominant mechanism leading to the new electron state is a redistribution of electrons in energy space induced by the direct current.

\(^1\)supported by NSF: DMR 0349049 and RFBR, project No.04-02-16789 and 06-02-16869.

9:00AM U37.00006 Influence of a Parallel Magnetic Field on the Microwave-Induced Resistance and Photovoltaic Oscillations, CHI ZHANG, KRISTJAN STONE, RUI-RUI DU, Rice University, CHANGLI YANG, Institute of Physics, CAS, China, LOREN PFEIFFER, KEN WEST, Bell Labs, Alcatel-Lucent — Microwave induced photovoltaic (PV) and resistance oscillations (MIRO) were studied in high-mobility (\(\mu > 8 \times 10^{7} \ cm^{2}/V \ s\) 2D electron gas in GaAs/Al\(_{0.33}\)Ga\(_{0.67}\)As Hall bar samples employing a two-axis magnet system (perpendicular field \(B_{\perp}\) and parallel field \(B//\). Consistent with the previous results, strong MIRO were observed and were found to diminish under a \(B//\sim\;1\;T\). We observed two types of PV oscillations: 1) PV oscillations that are periodic in \(1/B_{\perp}\), with a periodicity similar to MIRO, but are anti-symmetric with respect to \(B_{\perp} = 0\); and, 2) PV oscillations due to edge magnetoplasmon modes, which are periodic in \(B_{\perp}\) and are symmetric with respect to \(B_{\perp} = 0\). Characteristically, the \(1/B_{\perp}\) oscillations in PV were completely suppressed by a \(B//\sim\;1\;T\), whereas the \(B_{\perp}\)-periodic oscillations retain their main features even in \(B// \;= \;2\;T\). Experimental data and a brief discussion will be presented. The work at Rice was supported by NSF DMR-0706634.
9:12AM U37.00007 Microwave-Induced Resistance Oscillations in Non-Faraday Configurations, KRISTJAN STONE, ZHUOQUAN YUAN, RUI-RUI DU, Rice University, CHANGLI YANG, Institute of Physics, CAS, China, LOREN PFEIFFER, KEN WEST, Bell Laboratories, Alcatel-Lucent — The microwave-induced resistance oscillations (MIROR) are commonly observed in high-mobility GaAs 2D electron systems (2DES), typically using a Faraday configuration. In a Faraday configuration, the electromagnetic components (E_x and H_y) coincide with the 2DES plane. We explore MIROR in a microstrip line geometry, in which the dominant excitation component in the 2DES plane is H_y. Our samples were 100 or 200 μm wide Hall bars of very-high mobility (εc × 8 × 10^7 cm^2/Vs) GaAs/AlxGa1-xAs heterojunctions or quantum wells with electron density ranging from 2.1 × 10^{11} cm^{-2}. Microwaves from a tunable source (2 GHz - 40 GHz) were fed via a semi-rigid coax cable to the microstrip line over the length of the Hall bar. In a temperature range of 0.3 K – 2.0 K, we observed strong MIROR features. We studied the fractional MIROR using both the microstrip line and dipole antenna geometries. By increasing the power, MIROR features associated with high-mobility 2DES were presented. Experimental data as well as a brief discussion will be presented. The work at Rice was funded by NSF DMR-0706634.

9:24AM U37.00008 Low Temperature Scanning Hall Probe Microscopy of 2D Electron Nanostructures, ZHUOQUAN YUAN, YANHUA DAI, RUI-RUI DU, Rice University, L.N. PFEIFFER, K.W. WEST, Bell Labs, Alcatel-Lucent — Current distribution can provide key information on microscopic properties of 2D electron systems (2DES) in the regime of quantum transport. However, imaging coherent electron flow is proven to be experimentally challenging. We developed a method to image current distribution by using low temperature (0.3K), high spatial resolution (5 μm) scanning Hall probe. We imaged the local magnetic field component perpendicular to the 2DES in GaAs/AlGaAs samples, and then used Fast Fourier Transform (FFT) technique to recover the current distribution from the data of magnetic field. As an example, we will present the data and a brief discussion on imaging geometrical resonance in anti-dot lattices patterned on a very high mobility 2DES. The research at Rice was supported by NSF DMR-0706634.

9:36AM U37.00009 Spin-Orbit Interaction in High-κ Dielectric Gated Rashba-2D Electron Gas and Mesoscopic Rings, YANHUA DAI, ZHUOQUAN YUAN, KRISTJAN STONE, RUI-RUI DU, Physics and Astronomy, Rice University, MIN XU, PEIDE YE, Electrical and Computer Engineering, Purdue University — There is increasing current interest in the quantum interference effect in mesoscopic devices fabricated on a Rashba-2D electron gas (2DEG), where the spin-orbit interaction parameters can be tuned by a potential gate. We explore ring structures that use a gate consisting of thin (5nm-50nm) high-κ dielectric Al2O3 or HFO2 layer and nano-patterned metals. The 2DEG is provided by lattice-matched In0.52Al0.48As/GaAs quantum wells that have a typical electron density n of 1.5 × 10^{12}/cm^2 and mobility μ ≥ 2 × 10^5 cm^2/Vs. The dielectric material was grown by atomic layer deposition. We will present the gate characteristics of Hall bars as well as magnetic transport data from gated mesoscopic rings. The work at Rice is funded by NSF DMR-0706634. Reference: M. Konig et al. Phys. Rev. Lett. 96, 076804 (2006); T. Bergsten et al., Phys. Rev. Lett. 97, 196803 (2006); B. Grbic et al., Phys. Rev. Lett. 99, 176803 (2007).

9:48AM U37.00010 Novel interaction-induced magneto-oscillations in ac conductivity of 2D electron gas, TIGRAN SEDRAKYAN, University of Wisconsin-Madison, MIKHAIL RAIKH, University of Utah — We demonstrate that electron-electron interactions in a high-k dielectric 2D electron gas give rise to the oscillatory correction, δσ_{int}(ω), to the ac magnetoconductivity, σ(ω). Similarly to the conventional single-particle harmonics of the cyclotron resonance, the oscillating correction is periodic in ωc, where ωc is the cyclotron frequency. However, unlike the single-particle oscillations, which are periodic with ω, the interaction correction is periodic with ω^2. Oscillatory behavior of the interaction-induced magnetoconductivity develops at very low magnetic fields, ωc ≪ ω, at such fields the conventional harmonics are suppressed by the disorder. The underlying physical process of the new effect is double backscattering of an electron from the impurity-induced Friedel oscillations. Unlike the case of single-particle oscillations, the electrons travel only a small portion of the Larmor circle during the time ~ω^{-1} between the two backscattering events.

10:00AM U37.00011 Many-body local field corrections to spin Coulomb drag in a quasi-two-dimensional electron system, SAMVEL BADALYAN, Department of Radiophysics, Yerevan State University, 375025 Armenia and Department of Physics, University of Regensburg, 93040 Regensburg, Germany, CHANG SUB KIM, Department of Physics, Chonnam National University, 500-757 Gwangju, Korea, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri - Columbia, Missouri 65211, USA — We investigate the effect of exchange and correlation on spin Coulomb drag in a quasi-two-dimensional electron gas of finite transverse width. We find that the finite transverse width of the electron gas causes a significant reduction of the spin Coulomb drag. This reduction, however, is largely compensated by the enhancement coming from the inclusion of many-body local field corrections beyond the random phase approximation. Our calculations are in very good agreement with and confirm the experimental observations of the spin Coulomb drag by C. P. Weber et al., Nature, 437, 1330 (2005).

1 This work is supported by the Volkswagen Foundation, the DFG Grant Sonderforschungsbereich 689, and NSF Grant No. DMR-0313681.

10:12AM U37.00012 Evidence of Coulomb Drag between Anderson Insulators, KAREE ELSEYAD, JOHN CARINI, DAVID BAXTER, Indiana University — We report observations of Coulomb drag between 200 Angstrom thick co-sputtered insulating amorphous silicon-niobium alloy films, separated by a thin silicon-oxide barrier. An apparent linear-response regime for the transresistance is found to only exist over a narrow range of layer separations (∼100 Angstroms) and material parameters (niobium concentrations ∼ 7%) at low driving currents (∼1nA) and temperatures below ∼20 Kelvin. The temperature dependence, as well as the magnitude, of the transresistance in this regime is consistent with predictions for that between Anderson insulators with long ranged intra-layer Coulomb interactions, provided that the density of states of the silicon-niobium layers are taken to be that of effectively 3-dimensional systems. This is in contrast with measurements of the temperature dependence of the dc layer-conductivity in such bilayer systems, which suggest that transport should be effectively 2-dimensional at these energies. We will discuss the fabrication and characterization of bilayer samples, as well as possible explanations for the observed magnitude and temperature dependence of the transresistance.

10:24AM U37.00013 Scaling of thermoelectric voltage induced by microwave radiation at the boundary between two-dimensional electron systems, N. ROMERO KALMANOVITZ, I. HOXHA, Y. JIN, S.A. VITKALOV, M.P. SARACHIK, Physics Dept., City College of the City Univ. of New York, I.A. LARKIN, International Center of Condensed Matter Physics, Brasilia, T.M. KLAPWijk, Delft Univ. of Technology, Dept. of Applied Physics — We report measurements of the rectification of microwave radiation (0.7-20 GHz) at the boundary between two-dimensional electron systems created by a narrow gap split gate on a silicon surface for different temperatures, electron densities and microwave power. For frequencies above 4 GHz and different temperatures, the rectified voltage Vdc as a function of microwave power P can be collapsed onto a single universal curve Vdc = f∗(P∗) using two scaling parameters. The scaled voltage, Vdc, is a linear function of power, P∗, for small power and proportional to (P∗)^{1/2} at higher power. A theory is developed which attributes the observed voltage to the thermoelectric response associated with local heating by the microwave radiation of adjacent two-dimensional electron systems with different densities n₁ and n₂. Excellent quantitative agreement is obtained between theory and experiment. *The work at the City College of New York was supported by DOE grant DOE-FG02-84-ER45153. The work at International Center of Condensed Matter Physics, Brasilia, was supported by IBEM fund from Brazilian Ministry of Science and Technology.
thermopower as high as 1000
the coexistence of the large thermopower and the low resistivity in this material is that not just the density of states, the effective mass, nor the band width, but,

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intercalated. Recently, in Ref. 1 and 2, we proposed that the magnetism and the superconductivity can have the same root. Namely they can originate from the

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Work supported by NSF Grant No. DMR-0605652 and by the Boise State McNair Scholars Program.

Thursday, March 13, 2008 8:00AM - 11:00AM –
Session U38 DCMP: Focus Session: Ferroelectric Oxide Superlattices and Oxide Thermoelectrics
Morial Convention Center 230

8:00AM U38.00001 Thermoelectric response of Lanthanum-doped SrTiO₃ thin-films grown under various oxygen partial pressures , MATTHEW L. SCULLIN, Dept. of Materials Science and Engineering, University of California, Berkeley, CA 94720, JAYAKANTH RAVICHANDRAN, Dept. of Mechanical Engineering, University of California, Berkeley, CA 94720, MARK HUIJGEN, Dept. of Physics, University of California, Berkeley, CA 94720, CHONG-HO YU, Lawrence Berkeley National Labs, Berkeley, CA, 94720, SUBROTO MAJUMDAR, Lawrence Berkeley National Labs, Berkeley, CA, 94720, R. RAMESH, Dept. of Materials Science and Engineering, University of California, Berkeley, CA 94720 — Doped strontium titanate is a strong candidate for the next-generation high-Z bulk thermoelectric material due to both its wide tunability in transport properties and very large carrier effective mass. Thermoelectric thin-films of Sr₁₋ₓLaₓTiO₃₋₈ with various La content were grown via pulsed-laser deposition (PLD) on (001)-oriented LSAT substrates under various oxygen partial pressures. We find that electron transport is dominated by carriers from oxygen vacancies in samples grown at low po₂ < 10⁻⁶ Torr, and that thermopower as high as 1000 µV/K can be achieved even in heavily La-doped samples. Doping combinations that yield resistivities as low as 5 mΩ-cm yield power factors 300 K as high as 0.7 W/m-K, implying ZT

8:12AM U38.00002 “Pudding mold”-type band dispersion as the origin of large thermopower in Na₂CoO₂ , KAZUHIKO KUROKI, Dept. App. Phys.+Chem, Univ. Electro-Commum., RYOTARO ARITA, Cond. Mat. Theory Lab., RIKEN — Na₂CoO₂ is an interesting material in that it has large thermopower, non-trivial magnetic property, and becomes superconducting when water molecules are intercalated. Recently, in Ref. 1 and 2, we proposed that the magnetism and the superconductivity can have the same root. Namely they can originate from the peculiar band dispersion of 11g band. In this study, by using Boltzmann’s equation, we calculated the thermopower of this system. We found that the coexistence of the large thermopower and the low resistivity in this material is not just the density of states, the effective mass, nor the band width, but indeed again the peculiar “pudding mold”-type band dispersion of the 11g band which consists of a dispersive portion below the Fermi level and a dispersionless portion above the Fermi level[3].


8:24AM U38.00003 Thermoelectric properties of Bi₃Sr₂CoO₅ thin films grown by pulsed laser deposition, SHUHANG WANG¹, VENIMADHAV ADAYAM², SHENGMING GUO³, QI LI, XIAOXING XI¹, Department of Physics, The Pennsylvania State University, University Park, USA — Epitaxial and c-axis preferred oriented oxide thermoelectric Bi₃Sr₂CoO₅ thin films have been deposited on LaAlO₃ (100), A₁₂O₃(001) and fused silica substrates using pulsed laser deposition. At room temperature, the Seebeck coefficient and resistivity are of the order of 125 µV/K, 120 µV/K, 110 µV/K, 2 mΩ·cm and 3 mΩ·cm, 2 mΩ·cm, 2 mΩ·cm, 14 mΩ·cm for the films on LaAlO₃ (100), A₁₂O₃(001) and silica substrates respectively. A large negative in-plane magnetoresistance (MR) is observed in the films at low temperatures, with a MR reaching 41% at T=1.8 K in films on LaAlO₃ (100). We also observed a large bias current-dependent resistivity in the films at low temperature, which has been attributed to the suppression of spin-density-wave by electric field.

1 Also with Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA
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3 Also with Department of Physics, Tsinghua University, Beijing, China
4 Also with Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, USA

8:36AM U38.00004 Localization of holes at oxygen sites in a thermoelectric rhodate revealed by photoemission spectroscopy, ISHIDA YUKIARI, BABA TERUHISA, RIKEN SPRing-8 Center, EGUCHI RITSUKO, MATSUNAMI MASA-HARU, ISSP U. Tokyo, TAGUCHI MUNETAKA, CHAINAINI ASHISH, RIKEN SPRing-8 Center, SENBA YASUNORI, OHASHI HARIHIKO, JASRI/SPRING-8, OKAMOTO YOSHIIKO, ISSP U. Tokyo, TAKAGI HIDENORI, RIKEN, SHIN SHIK, RIKEN SPRing-8 Center & ISSP U. Tokyo — We have performed soft-x-ray absorption and photoemission studies on Sr₁₋ₓRh₂O₄⁺[1], a thermoelectric material structurally and electronically analogous to Na₅CoO₂. Metal-insulator transition occurs with hole doping into the Rh 4d t₂g band via introducing Sr vacancies [1]. Valence-band spectra of Sr₁₋ₓRh₂O₄ showed satellite structures ~11 eV below the Fermi level, which cannot be explained by LDA or LDA+U calculations. The O 1s 2p₂p Auger peak in the photoemission spectra appeared from the 11-eV satellite in the vicinity of the O 1s absorption edge, indicating that the satellite is a sign of holes localized at oxygen sites. Concomitantly, doping dependent changes appeared mainly in the O 1s absorption spectra rather than in the Rh 3p₃/2 absorption spectra. We discuss inhomogeneous evolution of the system with hole doping along with Sr-vacancy potential and d-p hybridization. [1] Y. Okamoto, et al., J. Phys. Soc. Jpn. 75, 023704 (2006).
10:12AM U38.00010 A new hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxide bulks and nanostructures , D.I. BILC, Université de Liège, Belgium, R. SHALTAF, Université Catholique de Louvain, Belgium, J. Íñiguez, Institut de Ciencia de Materials de Barcelona, Spain, PH. GHOSEZ, Université de Liège, Belgium — We report a systematic comparison of various DFT and hybrid exchange-correlation functionals for the prediction of the electronic and structural properties of prototypical ferroelectric oxides. We find that some, although not all, usual DFT functionals predict the structure with acceptable accuracy, but always underestimate the electronic band gaps. Conversely, common hybrids yield an improved description of the band gaps, but overestimate the volume and atomic distortions associated to ferroelectricity, giving rise to an unacceptably large c/a ratio for the tetragonal phases of BaTiO$_3$ and PbTiO$_3$. This super-tetragonality is found to be induced mainly by the GGA exchange energy. We thus propose an alternative hybrid functional, B1-WC, that mixes exact exchange following the B1 scheme with the recently improved GGA proposed by Wu and Cohen. This B1-WC renders accurate description of the both structural and electronic properties of typical ferroelectric oxide at the bulk level. The case of Pt/BaTiO$_3$ heterostructures is also considered and a comparison of the of B1-WC and LDA results for atomic relaxation and electronic band alignment at the interface is presented.

1In collaboration with Massimiliano Stengel, Karin M. Rabe and David Vanderbilt.

10:00AM U38.00009 Improper ferroelectricity in perovskite oxide artificial superlattices , MATTHEW DAWBER, NICOLAS STUCKI, CELINE LICHTENSTEIGER, JEAN-MARC TRISCONE, DPMC, University of Geneva, Switzerland, ERIC BOUS-QUET, PATRICK HERMET, PHILIPPE GHOSEZ, Physique Theorique des Materiaux, Université de Liège, Belgium — In paraelectric/ferroelectric heterostructures with thick constituent layers electrostatics is the dominant interaction between layers and we have previously demonstrated that the key ferroelectric parameters, polarization and critical temperature can be tuned over a very large range in PbTiO$_3$/SrTiO$_3$ superlattices by varying the ratio of the layer thicknesses [1]. However, as the layers become thinner, a departure from the electrostatic model is observed, which manifests itself as an unusually high ferroelectric polarization and transition temperature and a high, but temperature independent, dielectric constant. Detailed examination of the phase transitions with temperature reveals that along with these enhanced characteristics there is a fundamental change in the nature of the ferroelectricity. The microscopic origin of this change, a form of improper ferroelectricity, is revealed by first principles calculations to occur through a coupling of oxygen rotations and the polarization mismatch at the interfaces in the material. References: [1] M. Dawber et al., Adv. Mat. (2007)

1Now at: Physics and Astronomy, SUNY Stony Brook, USA
10:24AM U38.00011 First principles calculations at fixed dielectric displacement, MASSIMILIANO STENGEL, UCSB; DAVID VANDERBILT, Rutgers University; NICOLA SPALDIN, UCSB — With the experimental advances in growth and characterization of superlattices and thin-film capacitors based on ferroelectric perovskites, it is becoming more and more crucial to achieve a fundamental understanding of these structures by accurate first-principles modeling. Unfortunately, difficulties in the treatment of finite electric fields and macroscopic polarization in periodic systems — in particular when metallic electrodes are present — make the application of ab-initio techniques to such systems particularly challenging. To address these issues, we present here a method to perform first-principles calculations of periodic systems at a fixed value of the macroscopic dielectric displacement. This technique, which complements previously established strategies to fix \( E \) or \( \varepsilon \), provides a simple and natural way to explore the phase diagram of a ferroelectric system as a function of a single electrical order parameter. We demonstrate the power of our approach by computing the electrical equations of state for two symmetrical ferroelectric capacitors which are based on the same combination of materials, Au and BaZrO\(_3\), but are characterized by inequivalent interface geometries and stoichiometries. In particular, we use the information extracted from the centrosymmetric systems to accurately predict the electrical equation of state for an asymmetric capacitor of analogous composition.

10:36AM U38.00012 Broadband Permittivity Measurements of Ruddlesden-Popper \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) Thin Films, N. ORLOFF, W. TIAN, D. SCHLOM, J. BOOTH, I. TAKEUCHI — In order to explore the microwave dielectric response of \( \text{Sr}_2\text{TiO}_4\), \( \text{Sr}_3\text{Ti}_2\text{O}_9\), and \( \text{Sr}_4\text{Ti}_3\text{O}_{10} \) thin films, we have performed broadband in-plane quantitative complex permittivity(\( \varepsilon \)) measurements on \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) thin films in the frequency range 100Hz-40GHz. The films, of approximately 160 nm thickness, were fabricated by molecular beam epitaxy\(^1\), and standard lithographic techniques were used to define coplanar waveguide transmission lines and interdigitated capacitors using gold. We extracted \( \varepsilon \) from the measured complex S-parameters (0.1-40GHz) and the complex impedance (100Hz-.001GHz), which were measured at 70K, 150K, 200K, and 250K using a cryogenic probe station. We found that below \( \sim 10\text{GHz} \) the \( \varepsilon 's \) of these thin films were approximately constant with frequency: \( \varepsilon \approx 38\), 48, and 100 for \( \text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1} \) respectively. In addition, the measured value for \( \varepsilon \) of \( \text{Sr}_2\text{TiO}_4 \) is consistent with recent theoretical calculations\(^2\).

10:48AM U38.00013 Competing structural instabilities in Ti-based layered-perovskite-oxide superlattices\(^3\), SERGE NAKHMANSON, Argonne National Lab — Utilizing first-principles computational techniques, we have mapped out structural instabilities in the Ruddlesden-Popper homologous oxide superlattice families with a general chemical formula \( \text{A}_{n-1}\text{A}_n\text{Ti}_n\text{O}_{3n+1} \), \( \text{A} = \text{Sr}, \text{Ba}, \text{Pb} \) (perovskite-type block) and \( A' = \text{Sr} \) (rocksalt-type block), for \( n = 1-5 \). Our calculations show that each superlattice family has a unique set of “instability footprints” — including the ferroelectric, antiferroelectric and antiferrodistortive types — which may or may not have a strong coupling to epitaxial strain. Furthermore, the existence and strength of structural instabilities within each particular family change dramatically with an increasing number of perovskite-type layers \( n \), granting us wide flexibility to fine-tune the properties of these materials for various device applications or, e.g., for integration into composites with magnetic Ru- or Mn-based layered-perovskite-oxide compounds.

\(^1\) Work supported under contract No. DE-AC02-06CH11357 between UChicago Argonne, LLC and the Department of Energy.

Thursday, March 13, 2008 8:00AM - 11:00AM
Session U39 GSNP: Focus Session: Structure and Dynamics of Complex Networks
Morial Convention Center 231

8:00AM U39.00001 From network dynamics to human activity and mobility patterns, ALBERT-LÁSZLÓ BARABÁSI, Center for Complex Network Research and Dept. of Physics, Northeastern University; Center for Cancer Systems Biology, Dana Farber Cancer Institute. — The next challenge of network research is to go beyond the structure and quantify the dynamics of interconnected systems. A particular difficult facet of this research requires us to understand the temporal and spatial driving forces that govern social, technological and biological networks. In this talk I will focus on the dynamical mechanism that drive the activity of social networks. While none of us thinks of our daily activity pattern as random, most modeling efforts approximate human activity with fundamentally random spacial and temporal patterns. My purpose is to offer evidence of a series of significant deviations from this random expectation. I will talk about the bursty temporal character of human activity patterns and the travel patterns of individuals. I will show that both human activity and travel patterns are far more regular than the standard Poisson and diffusion models would predict, with implications on agent based models, epidemic modeling as well as the nature of time and space experienced by humans. The work was done in collaboration with Marta Gonzales, Cesar Hidalgo, Kwang-il Goh, Joao Oliveira, and Alexei Vazquez.

8:36AM U39.00002 Finite Size Effects and Symmetry Breaking in the Evolution of Networks of Competing Boolean Nodes\(^1\), KEVIN BASSLER, MIN LIU, University of Houston — The effects of finite network size on the evolutionary dynamics of a Boolean network are analyzed. In the model considered, Boolean networks evolve via a competition between nodes that punishes those in the majority. Finite size networks evolve in a fundamentally different way than infinitely large networks do. The symmetry of the evolutionary dynamics of infinitely large networks that selects for canalizing Boolean functions is broken in finite size networks. In finite size networks there is an additional selection for input inverting Boolean functions. Classes of functions are found empirically to evolve with the same frequency. The classes depend on the symmetry of the evolutionary dynamics and correspond to orbits of the relevant symmetry group. The empirical results match analytic results, determined by utilizing Polya's theorem, for the number of orbits expected in both finite size and infinitely large networks. The reason for the symmetry breaking is due to the need for nodes in finite size networks to behave differently in order to cooperate to collectively perform efficiently. The results suggest that both finite size effects and symmetry are important for understanding the evolution of real-world complex networks, including genetic regulatory networks.

\(^1\)Supported by the NSF through grant DMR-0427938.

8:48AM U39.00003 Attractors in continuous and Boolean networks\(^1\), JOHANNES NORRELL, JOSHUA SOCOLAR, Physics Department and Center for Nonlinear and Complex Systems, Duke University; BJÖRN SAMUELSSON, Lund University — Random Boolean models of complex regulatory networks are known to exhibit rich dynamical behaviors, including an order/disorder transition. We show that implementation of the nominal Boolean logic of a network using differential equations involving sigmoidal switching functions generically leads to deviations from the Boolean predictions. On simple rings, the “reliable” set of Boolean attractors corresponds to the stable attractors of the analogous continuous system. For networks with more complex logic, however, the set of the continuous attractors is determined by non-Boolean characteristics of the switching events. In large random networks, the nature of the order/disorder transition is altered by collective effects associated with compositions of the sigmoidal switching functions.

\(^1\)Supported by NSF.
9:00AM U39.00004 Scale-Free Overlay Topologies with Hard Cutoffs for Unstructured Peer-to-Peer Networks1, HASAN GUCLU, Los Alamos National Laboratory, MURAT YUKSEL, University of Nevada at Reno — The topology have profound impact on the efficiency of search on unstructured peer-to-peer (P2P) networks as well as other networks. It has been well-known that search on scale-free (power-law) topologies offer outstanding search efficiency as good as $O(\ln \ln N)$ for a range of degree distribution exponents. However, generation and maintenance of such scale-free topologies are hard to realize in a distributed and potentially uncooperative environments as in the P2P networks. A key limitation of scale-free topologies is the high load (i.e. high degree) on very few number of hub nodes. In a typical unstructured P2P network, peers are not willing to maintain high degrees/loads as they may not want to store large number of entries for construction of the overlay topology. So, to achieve fairness and practicality among all peers, hard cutoffs on the number of entries are imposed by the individual peers. Thus, efficiency of the flooding search reduces as the size of the hard cutoff does. Interestingly, we observe that the efficiency of normalized flooding and random walk search algorithms increases as the hard cutoff decreases.

1This work is supported by the U.S. DOE through Grant No. DE-AC52-06NA25396 and by the NSF grant No. 0627039.

9:12AM U39.00005 A Self–organized model for network evolution, GUIDO CALDARELLI, CNR-INFM Centre SMC Dip. Fisica, University “Sapienza” Rome, Italy, ANDREA CAPOCCI, Dip. Fisica Universita’ “Sapienza” Rome, Italy, DIEGO GARLASCHELLI, Dipartimento di Fisica, Università di Siena, Italy — Here we present a self-organized model for the evolution of complex networks. Vertices of the network are characterized by a variable evolving through an extremal dynamics process. The network topology is in turn shaped by the variable itself. More specifically, to each vertex a fitness is assigned; then, in the evolution, the vertex with minimum fitness and its neighbors are updated by extracting new fitesses. For any given realization of fitnesses we can determine the edges in the network through a fitness dependent rule. We show analytically and numerically that this system self-organizes to a nontrivial state. A power–law decay of dynamical and topological quantities above a threshold emerges spontaneously, as well as a feedback between different dynamical regimes and the underlying network’s correlation and percolation properties.

9:24AM U39.00006 Money circulation networks reveal emerging geographical communities, D. BROCKMANN, MPI-DS, Goettingen, Germany & Northwestern University, F. THEIS, CMB, Institute for Bioinformatics, Neuherberg, Germany, V. DAVID, MPI-DS, Goettingen, Germany — Geographical communities and their boundaries are key determinants of various spatially extended dynamical phenomena. Examples are migration dynamics of species, the spread of infectious diseases, bioinvasive processes, and the spatial evolution of language. We address the question to what extend multiscale human transportation networks encode geographical community structures, how they differ from geopolitical classifications, whether they are spatially coherent, and analyse their structure as a function of length scale. Our analysis is based on a proxy network for human transportation obtained from the geographic circulation of more than 10 million dollar bills in the United States recorded at the bill tracking website www.wheresgeorge.com. The data extends that of a previous study (Brockmann et al., Nature 2006) on the discovery of scaling laws of human travel by an order of magnitude and permits an approach to multiscale human transportation from a network perspective.

9:36AM U39.00007 Functional structure through dynamic clustering of neuronal networks1, SARAH FELDT, MICHAL ZOCOWSKI, University of Michigan — We propose a new method for detecting functional structure in neuronal networks based solely upon the information derived from the spike timings of the neurons. Unlike traditional algorithms that depend on knowledge of the topological structure of the network to parse the network into communities, we dynamically cluster the neurons to build communities with similar functional interactions. We define means to derive optimal clustering parameters and investigate what conditions have to be fulfilled to obtain reasonable predictions of functional structures.

1Supported through an NSF Graduate Research Fellowship and NIH Grant EB005583.

9:48AM U39.00008 Citation analysis: Beyond the Journal Impact Factor, MANOLIS ANTONOYIANNAKIS, (1) Physical Review Letters (2) Columbia University — The journal impact factor is a robust measure of the average citation performance of a journal, but the number of citations varies widely from paper to paper within any journal. Therefore, it makes sense to look for additional ways of characterizing journals in terms of their impact. We introduce the “citation density curve” (citations per paper in a given year for papers published in the previous two years, plotted vs. the citation rank of these papers). This curve, which displays a Zipf’s law behavior, contains all the pertinent information about a journal: its size, its impact factor, the maximum number of citations per paper, the relative size of the top-cited portion of the journal, how the citation density varies within the journal, etc. Being the “fingerprint” of a journal, the citation density curve can be used: (a) by editors, for strategic decisions affecting the future of their journal; (b) by citation analysts, for comparing (ranking) journals; and (c) by authors, for assessing the relative impact of their published work. Further, we identify a complementary metric to the impact factor, a single number that characterizes the top-cited portion of a journal. This metric reproduces the ranking of the citation density curves for various journals, and can be readily calculated from the same data used in the impact factor calculations. We propose that this new metric be used as an essential complement to the impact factor in assessing the true impact of journals.

10:00AM U39.00009 Epidemics on adaptive networks with geometric constraints, LEAH SHAW, College of William and Mary, IRA SCHWARTZ, Naval Research Lab — When a population is faced with an epidemic outbreak, individuals may modify their social behavior to avoid exposure to the disease. Recent work has considered models in which the contact network is rewired dynamically so that susceptibles avoid contact with infectives. We consider extensions in which the rewiring is subject to constraints that preserve key properties of the social network structure. Constraining to a fixed degree distribution destroys previously observed bistable behavior. The most effective rewiring strategy is found to depend on the spreading rate.

10:12AM U39.00010 Some aspects on human preference in communication and friendship, DIEGO RYBSKI, HERNAN D. ROZENFELD, Levich Institute and Physics Department, City College of New York, New York, NY 10031, USA, FREDRIK LILJEROS, Department of Sociology, Stockholm University, S-106 91 Stockholm, Sweden, SHLOMO HAVLIN, Minerva Center and Department of Physics, Bar-Ilan University, 52900 Ramat-Gan, Israel, HERNAN A. MAKSE, Levich Institute and Physics Department, City College of New York, New York, NY 10031, USA — The objects of our investigation are social networks consisting of individual actants as nodes and their relations as links. Recently, on-line communities have gained immense popularity as indicated by millions of members participating in these platforms. Fortunately, the information given by member activity provides an ideal environment to study structural preferences of social behavior. In particular, we address the questions of how network topology benefits the spreading rate.

Among others, we find that actants tend to get connected at a distance of 2. Further analysis indicates that the more common neighbors two actants have, the more likely they will be in relation with each other. We attribute this behavior to some kind of social pressure imposed by the neighborhood biasing the actants preferences.
10:24AM U39.00011 Studying Human Dynamics Through Web Analytics, JOSE RAMASCO, I.S.I., Torino, Italy, BRUNO GONCALVES, Emory University, Atlanta Ga, 30322 — When Tim Berners Lee, a physicist at the European Center for Nuclear Research (CERN) first conceived the World Wide Web (WWW) in 1990 as a way to facilitate the sharing of scientific information and results among the centers different researchers and groups, even the most ingenious of science fiction writers could not have imagined the role it would come to play in the following decades. The increasing ubiquitousness of Internet access and the frequency with which people interact with it raise the possibility of using it to better observe, understand, and even monitor several aspects of human social behavior. Websites with large numbers of frequently returning users, such as search engines, company or university websites, are ideal for this task. The properly anonymized logs detailing the access history to Emory University’s website is studied. We find that a small number of users is responsible for a finite fraction of the total activity. A saturation phenomenon is observed where, certain connections age, becoming less attractive to new activity over time. Finally, by measuring the average activity as a function of the day of the week, we find that productivity seems to be higher on Tuesdays and Wednesdays, with Sundays being the least active day.

10:36AM U39.00012 Which Route Will You Choose to Use For Driving Home Tonight in Rush-Hour Traffic?1, BOGDAN DANILA, YUDONG SUN, KEVIN BASSLER, University of Houston — The best answer to the question posed in the title for a city of drivers requires knowing the optimal routes for congested traffic flow on complex networks. This is known to be an NP-hard problem. Despite this fact, we can arrive at optimal answers in integral polynomial time using extensions of a recently introduced heuristic algorithm [Danila, et al., PRe 74, 046106 (2006)] that, at least, scale optimally with network size. Using the optimal routes allows a network to support the maximum traffic load and significantly reduces the average travel time in congested traffic. The results presented apply to vehicular traffic and to traffic on wireless communication networks.

Thursday, March 13, 2008 8:00AM - 11:00AM
Session U40 DBP: Biomolecular Computation Morial Convention Center 232

8:00AM U40.00001 Hydrophobic polymers in nano-sized water droplets, BUDDHI TILAKARATNE, University of Houston, SAMINA MASOOD, University of Houston, CLEAR LAKE, MARGARET CHEUNG, University of Houston — As simulations of biopolymers take place in confined and tight spaces, such as protein folding in the interior of bacteria chaperones or the exit tunnels of ribosomes, quantitative analyses of the confinement effects on both biopolymers and solvent molecules become the center of attention as the solvent-mediated interactions are too profound to solve analytically. We are in the progress to investigate the solvation of hexane molecules in various nano-sized water droplets. Free energy profiles for a single hexane molecule in droplets show that the droplet surfaces are favored. Averaged configurations of hexane molecules at the interior and the surface are computed using the umbrella sampling methods. The implications of our results for protein stability in confined spaces will be discussed.

8:12AM U40.00002 A classical density functional for water, DAVID ROUNDY, DENNIS JACKSON, Oregon State University — We present a classical density functional for water that represents the short-range repulsive interaction using the fundamental-measure-theory hard-sphere functional. The parameters of this functional are chosen to reproduce the experimental liquid density, bulk modulus and surface tension of water, and to ensure coexistence of liquid and vapor phases. This functional inherits from the FMT functional its accurate description of reduced-dimensionality configurations. We will present computations of the hydrophobic hydration energy of hard-sphere solutes, demonstrating an accurate description at both large and small length scales.

8:24AM U40.00003 Hydrophobic interactions at molecular scale, DUBRAVKO SABO, SAMEER VARMA, SUSAN REMPE, MARCUS MARTIN, Sandia National Laboratories — Structural and thermodynamic properties are investigated for one of the simplest hydrophobic solutes, a hydrogen molecule solvated in liquid water. The structural properties are calculated using different representations of the intermolecular interactions within molecular dynamics, Monte Carlo and ab initio molecular dynamics simulation frameworks. Although structural details differ in the radial distribution functions obtained by different force fields all approaches agree that 16 water molecules coordinate hydrogen. The thermodynamic properties are investigated using Monte Carlo molecular simulation and the quasichemical theory of liquids. Results show that the net hydration free energy arises from a balance between chemical association and molecular packing. Additionally, the results suggest the molecular packing is almost equally driven by unfavorable enthalpic and entropic components.

8:36AM U40.00004 Computing absolute binding affinities via non-equilibrium unbinding simulations, F. MARTY YTBREBERG, University of Idaho — We demonstrate that non-equilibrium unbinding simulations can be used to accurately estimate equilibrium absolute binding affinities (ΔG). Utilizing the FKBP protein bound to two different ligands we estimate ΔG within less than 1.0 kcal/mol of experimental values. The methodology is straightforward, requiring no modification to many modern molecular simulation packages. The approach makes use of a physical pathway, eliminating the need for complicated alchemical decoupling schemes. These results suggest that non-equilibrium simulation could provide a viable means to accurately estimate protein-ligand binding affinities.

8:48AM U40.00005 Macromolecular crowding effects on Brownian motion of protein GB1, ANTONIOS SAMIOTAKIS, MARGARET CHEUNG, University of Houston — The effect of macromolecular crowding in the interior of a cell plays an important role in protein folding dynamics and its stability. In the present work the dependence of diffusion coefficients of the macromolecule on various crowding conditions is studied using a coarse-grained representation of protein G B1 domain that includes Go-like interactions. Using Brownian dynamics simulations, diffusion coefficients are computed as a function of the volume fraction of crowders φc and the ratio λ of the sizes of the crowder over that of protein. Deviation from linear Stokes-Einstein relation will be discussed.
9:00AM U40.00006 Core-Shell Model of Folding-Unfolding Transitions (UFT) in Proteins

SVETLANA AROUTIOUNIAN — There are ~10^N conformations for a protein of length N to sort out randomly in search of lowest free energy state. Can protein folding be simple and fast? Core-shell model introduces principles, proposes mechanisms and scores residues of fast, reversible UFT in protein. According to it, during UFT the realm of intra-residual interactions leads the residue motion. The scaffold of hydrophilic residues forms external shell of unstructured, tube-like protein in unfolded state, just as the hydrophobic residues form internal scaffold — core, of the protein in folded state. As UFT proceeds, residue slides into lowest-score position permitted by its structure. Model accounts for experimentally observed features of UFT. It is based on three principles: 1) During UFT protein is virtual - its features or structure are inferred only statistically and with limited precision; 2) Mechanism of UFT memory is not longitudinal, but transverse; 3) Native design overrides specific features of residues - the alphabet of amino acids becomes score-function. Per-residue mechanism of UFT is proposed and score-function is described. Difference graphs of transitional score-function and average genome-wide abundance index show that our score-function is the order parameter of UFT in protein and as virtue of being it, reveals transitional key residues. It echoes the multiple-tier and funnel concepts of FEL perspective. Monte Carlo simulations of UFT in myoglobin illustrate the idea.

9:12AM U40.00007 Potential of mean force of Glycophorin A alpha-helix dimerization

LORANT JANOSI, MANOLIS DOXASTAKIS, University of Houston — Transmembrane proteins recognition and association plays a crucial role in their assembly and function. In spite of the extensive studies, these processes are only partially understood. We investigate the association of the model transmembrane alpha-helices by means of coarse-grained simulations with reference interaction site model theory for simulating proteins in aqueous solution. The reference interaction site model theory based on the liquid theory of statistical mechanics can treat solvent effect with solvent molecular shape and estimate solvation free energy around proteins. We have developed simulation algorithms which combine with generalized-ensemble algorithms and reference interaction site model theory. We showed results of a simulated annealing Monte Carlo simulation, a multicanonical Monte Carlo simulation, and a replica-exchange Monte Carlo simulation with one dimensional reference interaction site model theory for Met-Enkephalin, a penta-peptide [1,2,3]. Recently we have performed a Monte Carlo simulation with three-dimensional reference interaction site model theory for simulating C-peptide in aqueous solution. We will describe these attempts and discuss results of these simulations.


9:24AM U40.00008 Monte Carlo Simulations with reference interaction site model theory for simulating peptide molecules in aqueous solution

AYORI MITSUTAKE, Keio Univ., YUTAKA MARUYAMA, IMS, TAKASHI IMAI, Ritsumei Univ., MASASHI KINOSHITA, Kyoto Univ., YUKO OKAMOTO, Nagoya Univ., FUMIO HIRATA, IMS — We have developed Monte Carlo simulations with reference interaction site model theory for simulating proteins in aqueous solution. The reference interaction site model theory based on the liquid theory of statistical mechanics can treat solvent effect with solvent molecular shape and estimate solvation free energy around proteins. We have developed simulation algorithms which combine with generalized-ensemble algorithms and reference interaction site model theory. We showed results of a simulated annealing Monte Carlo simulation, a multicanonical Monte Carlo simulation, and a replica-exchange Monte Carlo simulation with one dimensional reference interaction site model theory for Met-Enkephalin, a penta-peptide [1,2,3]. Recently we have performed a Monte Carlo simulation with three-dimensional reference interaction site model theory for simulating C-peptide in aqueous solution. We will describe these attempts and discuss results of these simulations.

9:36AM U40.00009 Glassy protein dynamics and gigantic solvent reorganization energy of plastocyanin

DAVID LEBERD, DMITRY MATYUSHOV, Center for Biological Physics, Arizona State University — This work focuses on the results of extensive explicit solvent Molecular Dynamics simulations of plastocyanin, a blue copper electron transfer protein involved in natural photosynthesis. Simulation data indicate that low-frequency non-ergodic fluctuations of the protein matrix tethered to the hydrating water are responsible for a very broad distribution of the vertical energy gaps of one-electron protein reduction/oxidation. The width of the corresponding free energy surfaces yields a reorganization free energy far larger than previously reported for any organic, inorganic, or biological chromophores. However, the Stokes shift is not affected by these slow motions and can be calculated from the polarization response function of the dipolar solvent using microscopic solvation models. The glassy nature of the protein-solvent interface breaks the direct link between the Stokes shift and the reorganization energy from equilibrium (ergodic) electron transfer theories. This suggests a mechanism that accounts for electron transfer in natural proteins, which are characterized by a low reaction free energy combined with a low activation barrier.

9:48AM U40.00010 Modeling low frequency vibrational modes of large biomolecules

OTT0 SANKEY, ERIC DYKEMAN, Arizona State University — Mechanical oscillations of proteins in their native state are relevant to understanding the flexibility of the protein assembly, the binding of substrates, the mechanical action involved in enzymatic activity, and the vibrational response to light scattering. Often, only the low frequency modes are of interest and coarse grained methods or other approximations are used due to the large size of the dynamical matrix. We introduce a computational approach, which exploits the methodology from electronic structure Order N methods, to find the vibrational modes below some high frequency threshold (analogous to a Fermi-level in electronic structure theory). The approach allows systems to be described in atomistic detail. We use a generalized Born force field to model the interactions. Examples of normal modes for icosaheiral viruses (e.g. satellite tobacco necrosis virus), tubular viruses (e.g. M13), and enzymes (e.g. lysozyme, HIV-protease, alpha-lytic protease) will be discussed. This effort is motivated by recent experimental work to produce high amplitude vibrations of viruses from impulsive stimulated Raman scattering.

10:00AM U40.00011 Monte Carlo simulations of Protein Adsorption

SUMIT SHARMA, SANAT K. KUMAR, Columbia University, GEORGES BELFORT, Rensselaer Polytechnic Institute — Amyloidogenic diseases, such as, Alzheimer’s are caused by adsorption and aggregation of partially unfolded proteins. Adsorption of proteins is a concern in design of biomedical devices, such as dialysis membranes. Protein adsorption is often accompanied by conformational rearrangements in protein molecules. Such conformational rearrangements are thought to affect many properties of adsorbed protein molecules such as their adhesion strength to the surface, biological activity, and aggregation tendency. It has been experimentally shown that many naturally occurring proteins, upon adsorption to hydrophobic surfaces, undergo a helix to sheet or random coil secondary structural rearrangement. However, to better understand the equilibrium structural complexities of this phenomenon, we have performed Monte Carlo (MC) simulations of adsorption of a four helix bundle, modeled as a lattice protein, and studied the adsorption behavior and equilibrium protein conformations at different temperatures and degrees of surface hydrophobicity. To study the free energy and entropic effects on adsorption, Canonical ensemble MC simulations have been combined with Weighted Histogram Analysis Method (WHAM). Conformational transitions of proteins on surfaces will be discussed as a function of surface hydrophobicity and compared to analogous bulk transitions.

10:12AM U40.00012 Complexation of Flavonoids with Iron: Structure and Optical Signatures

JUN REN, SHENG MENG, Physics Department and School of Engineering and Applied Sciences, Harvard University, CH. E. LEKKA, Department of Materials Science and Engineering, University of Ioannina, Ioannina 45110, Greece, EFTHIMIOS KAXIRAS, Physics Department and School of Engineering and Applied Studies, Harvard University — Flavonoids exhibit antioxidant behavior believed to be related to their metal ion chelation ability. We investigate the complexation mechanism of several flavonoids, quercetin, luteolin, galangin, kaempferol and chrysin with iron, the most abundant type of metal ions in the body, through first- principles electronic structure calculations based on Density Functional Theory (DFT). We find that the most likely chelation site for Fe is the 3-hydroxyl-4-carbonyl group, followed by 4- carbonyl-5-hydroxyl group and the 3’-4’ hydroxyl (if present) for all the flavonoid molecules studied. Three quercetin molecules are required to saturate the bonds of a single Fe ion by forming six orthogonal Fe-O bonds, though the binding energy per molecule is highest for complexes consisting of two quercetin molecules and one Fe atom, in agreement with experiment. Optical absorption spectra calculated with time-dependent DFT serve as signatures to identify various complexes. For the iron-quercetin complexes, we find a redshift of the first absorbance peak upon complexation in good agreement with experiment; this behavior is explained by the narrowing of the optical gap of quercetin due to Fe(d)–O(p) orbital hybridization.
10:24AM U40.00013 When Cells Collide: A Model for Cell-Assisted Cell Growth based on Direct Contacts. CARL FRANCK, WUI IP, ALBERT BAE, NATHAN FRANCK, ELIJAH BOGART, THANHBINH THI LE, Cornell University — Although intercellular communication is frequently viewed as involving the transport of small molecules through an intracellular fluid medium, biologists have proposed chemical signaling with chemical specificity due to chemical recognition through direct contacts. Considering the collective computation behind the decision of a cell to divide when it senses the presence of a sufficient number of like neighbors, we offer a model for the transition from slow to exponential growth in shaken suspension cell culture of the model eukaryote, Dictyostelium discoideum. Besides exploring an elegantly simple example of multicellular life, this discussion might well prove useful in considering the limits of cell culture on small spatial scales as required for contemporary massively parallel biotechnology.

10:36AM U40.00014 Do Porins Pass CAPs?1, C.B. HANNA, Boise State University, D.A. PINK, St. Francis Xavier University, T.A. GILL, Dalhousie University, T.J. BEVERIDGE, University of Guelph, B.E. QUINN, J.J. DURRANT, Boise State University, M.H. JERICHO, Dalhousie University — The cationic antimicrobial peptide (CAP) protamine is known to inhibit bacterial survival (Pink et al., Langmuir 19, 8852 (2003), and references therein), but the mechanism of attack is as yet undetermined. For Gram-negative bacteria, two pathways have been proposed: (a) self-promoted uptake, and (b) passage through porins. Here, we study the latter possibility, and model part of the outer membrane of a Gram-negative bacterium in an aqueous solution containing multivalent ions and CAPs. The intent is to determine whether CAPs could pass through porins and, if so, what aspects of external (e.g., ionic concentration) and internal (e.g., porin and O-sidechain characteristics) parameters affect their passage. This study is accomplished via Monte Carlo computer simulations of a “minimal model” of the outer membrane of a Gram-negative bacterium with an embedded porin.

Parameterization of Regional and Global Features. CLAYTON BRATTON, Dept.of Physics, Univ. of California, Davis, KAREN REISER, Dept.of Neurological Surgery, Univ. of California, Davis, ANDRE KNOESEN, DIEGO YANKELEVICH, MINGSHI WANG, Dept. of Electrical and Computer Eng., Univ. of California, Davis, ISRAEL ROCHA-MENDOSA, Cardiff School of Biosciences, Univ. of Cardiff, Wales — We have continued development of our novel computational approach for quantifying structural disorder in biomolecular lattices with nonlinear susceptibility based on analysis of polarization-modulated second harmonic signal. Local disorder at the level of molecular organization is identified using a novel signal-processing algorithm sufficiently compact for near real-time analysis. Global and regional disorder within the biostucture is characterized using two-dimensional wavelet transform of the magnitude and phase of the second harmonic signal. Results suggest our signal processing method represents a robust, scaleable tool that allows us to detect both regional and global alterations in signal characteristics of biestructures with a high degree of discrimination.


11:15AM V1.00001 Neutron and X-ray Characterization of Nanostructured Polymeric Materials1. THOMAS RUSSELL, Polymer Science and Engineering Department, University of Massachusetts, Amherst, MA 01003 Amherst — Controlling the orientation and lateral ordering of the block copolymer microdomains is key to their use as templates and scaffolds for the fabrication of nanostructured materials. Processes must be robust, rapid and simple to implement and should not introduce disruptive processing steps that would impede their use. Grazing incidence small angle x-ray scattering (GISAXS) and neutron neutron scattering have proven to be critical for the characterization of the static and real time development of structure in thin films of block copolymers. Here, studies on poly(styrene-b-4-vinylpyridine) (PS-b-P4VP) diblock copolymers prepared from mixed solvents will be discussed that show highly oriented, cylindrical microdomains with a high degree of lateral order on a wide range of substrates, including silicon oxide, polystyrene, germanium, polyimide, and polyl butylene terephthalate). The preferential solvation of the P4VP block with an alcohol was used to induce a reconstruction that left a nanoporous film upon drying. The evaporation of gold onto the reconstructed films produced thermally stable films that are resistant to reactive ion etching. GISAXS was used to quantitatively examine the structure of these composite films and the transfer of the patterns to the underlying substrate. (Research done in collaboration with Soojin Park, Jia-Yu Wang, Bokyung Kim University of Massachusetts, Benjamin Ocko (Brookhaven National Laboratory) and Jin Wang (Argonne National Laboratory).

1 DOE BES; NSF MRSEC

11:51AM V1.00002 Beyond Wrinkles: Stress and Fold Localization in Thin Elastic Membranes1. LUKA POČIVAVŠEK, University of Chicago — Thin elastic membranes supported on fluid or elastic foundations deviate from their flat geometries upon compression. We demonstrate that the periodic and much studied wrinkled state is but one possible solution for such strained membranes. Folds, sharply localized solutions, appear whenever the membrane is compressed beyond a third of its initial wrinkle wavelength. Eventually the surface transforms into a symmetry broken state with flat regions of membrane coexisting with locally folded points, reminiscent of a crumpled unsupported membrane. We study this transition in many systems including lipid monolayers on liquid subphases of differing viscosity and use neutron and X-ray reflectivity to elucidate the role of the subphase in setting the wrinkle and fold size.

1 UChicago MRSEC

12:27PM V1.00003 Complex Protein Structures by Neutron Scattering1. JENNY GLUSKER, Fox Chase Cancer Center, 333 Cottman Avenue, Philadelphia, PA 19111-2497 — Neutron scattering by an atom, unlike X-ray scattering, does not depend on the atomic number of that atom. Deuterium atoms scatter neutrons to the same extent as carbon or oxygen atoms and give positive peaks in a nuclear density map, while its isotope, hydrogen, gives a negative peak. Therefore neutron diffraction provides two results that are difficult to obtain from macromolecular X-ray diffraction studies: (1) the locations of hydrogen atoms, including the more mobile ones, and (2) the extent to which a hydrogen atom can be replaced by deuterium. For example, one can ascertain whether histidine residues are singly or doubly protonated at the pH of study. Neutron diffraction studies can also be used to determine the absolute configuration of the course of a biochemical reaction by anomalous scattering and enzymatic deuterium of the substrate. Neutron diffraction experiments, however, require large crystals and these are often impossible to obtain for many macromolecules. Examples of reports of the use of neutron diffraction to provide information on enzymatic mechanism will be presented. This includes discriptions of our work on the enzyme D-xylene isomerase for which the orientation of a metal ion-bound water molecule in the active site was found. This water, thought to be involved in the isomerization step, was shown to be water (rather than hydroxyl) at pH 8.0. This analysis also revealed that one lysine has two rather than three attached hydrogen atoms and therefore lacks a positive charge. High-resolution X-ray studies (at 0.94 Å) indicate how some side chains might move during catalysis. This combination of neutron and X-ray diffraction can contribute greatly to the elucidation of enzyme mechanisms. I thank Amy Katz, Xinmin Li, H. L. Carrell, Leighton Coates, Leif Hanson, Joel Haprl, Paul Langan, and Benno Schoenborn who were involved in many of the described studies, and particularly Gerard Bunic. We honor his contributions and regret that he is no longer with us.

1National Institutes of Health grant numbers CA-10925 and CA-06927.
1:03PM V1.00004 Observation of a Fragile-to-Strong Dynamic Crossover Phenomenon in Confined Water and Its Relation to the Existence of a Liquid-Liquid Critical Point in Supercooled Water, SOW-HSIN CHEN, Massachusetts Institute of Technology — We have observed a fragile-to-strong dynamic crossover phenomenon of α relaxation time and self-diffusion constant in deeply supercooled 1-d confined water. The α relaxation time is measured by quasi-elastic neutron scattering and the self-diffusion constant by nuclear magnetic resonance. Water is confined in 1-d geometry in cylindrical pores of porous silica material, MCM-41 and in double-wall carbon nanotubes. The crossover phenomenon can also be observed from appearance of a Boson peak in incoherent inelastic neutron scattering. We observe a pronounced violation of the Stokes-Einstein relation at and below the crossover temperature at ambient pressure. Upon applying pressure to the confined water, the crossover temperature is shown to track closely the Widom line emanating from the existence of a liquid-liquid critical point buried in an unattainable deeply supercooled state of bulk water. Relation of the dynamic crossover phenomena to the existence of a density minimum in supercooled confined water will be discussed. The crossover temperature is shown to be sensitively dependent on the degree of hydrophilicity of the confining substrate.

1:39PM V1.00005 Phase Behavior of Block Copolymer/Inorganic Nanoparticle Composites, PAPPANAN THIYAGARAJAN, Argonne National Laboratory — Block copolymers offer as versatile platforms for the fabrication of hybrid nanocomposites with ordered phases useful for various nanotechnology applications. Although the phase behavior of block copolymers is well established the effects of inorganic nanoparticle loading on their phase behavior are not well understood. We carried out a systematic study on the phase behavior of block copolymers with well dispersed nanoparticles. To achieve excellent dispersion of nanoparticles in the polymer phase we used grafted nanoparticles with small polymer chains compatible to a preferred domain of the block copolymer. The nanoparticles sequestered in a preferred domain have profound effects on the thermodynamically induced microphase separation of the block copolymers. To characterize the phase behavior of these systems in a selective solvent we used small angle neutron scattering and that in their bulk and thin film architectures was studied using synchrotron based small angle x-ray scattering and grazing incidence small angle scattering techniques. A number of molecular properties such as the molecular weight of the polymer, segment volume fraction, Flory-Huggins χ parameter and the nanoparticle concentration influence the state of dispersion of nanoparticles and the nanocomposite morphology in bulk and thin film architectures. The addition of homopolymers provides as yet another variable to alter the interfacial tension and to slow the order-disorder transition. We also probed the nanoscale dynamics at the polymer/nanoparticle interfaces in these systems by using x-ray photon correlation spectroscopy. The dynamics of nanoparticles in the composites is strongly dependent on the dimensionality of the morphology of the block copolymer. Furthermore, the interfacial interaction at the polymer/particle interface plays significant role in the stress relaxation in the composites.

Thursday, March 13, 2008 11:15AM - 1:39PM — Session V2 DCMP GIMS: Facilities for Meeting Grand Challenges  
11:15AM V2.00001 A Green Field Fourth Generation Light Source1, GEORGE NEIL, Jefferson Lab — The success of energy recovering linac technology has opened up new opportunities for the development of light sources to satisfy grand challenges in fundamental physics and materials research. A number of laboratories around the world have proposed extensions or upgrades to existing 2nd or 3rd generation light source facilities to take advantage of the higher brightness and short pulse lengths that 4th generation facilities could offer. Ideas range from multiple synchronized coherent sources in the THz to UV range to Compton X-ray sources, synchrotron emission, and on to achievement of multi-particle coherence in amplifiers or even oscillators at short wavelengths. Such proposals are exciting and begin to show the range of performance that such systems can provide. In this talk I will examine the possibilities for light source development unconstrained by existing physical layouts i.e., on a “green field” site. I will then address a set of photonic goals to be achieved and the technological path of development desirable to achieve the full benefits of this next generation of user facilities. In particular, there are specific technical achievements and engineering developments with great leverage on the cost and performance of future machines. I will point toward a development path to set the stage for optimization of technical performance and cost/benefit of this system.

1 Notice: Authored by The Southeastern Universities Research Association, Inc. under U.S. DOE Contract No. DE-AC05-84ER40150. The U.S. Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce this manuscript.

11:51AM V2.00002 Science Driven the Parameters of 4th Generation Light Sources, JEROME HASTINGS, Stanford Linear Accelerator Center — The scientific challenges that can be best addressed with x-rays and the evolution of accelerator based x-ray sources has focused the attention of the x-ray community on new concepts: using the electron beam once rather than storage rings. We will describe this approach and the photon source properties that result with emphasis on peak and average brightness for the study of structure and dynamics in the chemical, materials and biological sciences. Examples from 4th generation sources planned and under construction will be presented.

12:27PM V2.00003 The Science Motivating the UK’s Fourth Generation Light Source Project, WENDY FLAVELL, The University of Manchester — The UK is committed to developing a proposal for a long wavelength (THz - soft X-ray) 4th generation light source that will provide short-pulse synchronised beams to be used in combination. Some of the science motivating the development of this facility is described. The facility will probe ultra-fast dynamics in a wide range of fields. ‘Pump-probe’ experiments will allow the study of chemical reactions and short-lived intermediates on the timescale of bond formation, even for very dilute species. Circularly polarised light sources in a variety of frequency regimes will be used for example to manipulate and monitor carrier charge and spin transport in device structures. The high intensity of the free electron laser (FEL) radiation will allow high resolution in imaging and the opportunity to probe nonlinear regimes and new states of matter. Lower intensity, high repetition rate spontaneous radiation will provide ideal sources for ultra-high energy resolution spectroscopy, especially in the solid state. Around £22 M funding has been obtained for the first stages of the project (construction of a prototype energy recovery linac (ERL) source, science demonstrations and design study work, currently underway at STFC Daresbury Laboratory).
11:15AM V3.00001 Industrial Research at IBM. PAUL HORN, IBM T.J. Watson Research Center — No abstract available.

11:51AM V3.00002 Reflections on Three Corporate Research Labs: Bell Labs, HP Labs, Agilent Labs. JAMES HOLLENHORST, Agilent Technologies — This will be a personal reflection on corporate life and physics-based research in three industrial research labs of the past three decades, Bell Labs during the 1980’s, HP Labs during the 1990’s, and Agilent Labs during the 2000’s. These were times of great change in all three companies. I’ll point out some of the similarities and differences in corporate cultures and how this impacted the research and development activities. Along the way I’ll mention some of the great products that resulted from physics-based R&D.

12:27PM V3.00003 Application Oriented R&D: Aphorisms & Anecdotes (The John Bardeen Lecture). ROBERT FROSCH, John F. Kennedy School of Government, Harvard University — I have learned many lessons from long experience trying to perform, and lead, application oriented R&D. Some of these lessons have been encapsulated in aphorisms. Some aphorisms will be presented, with explication, and illustrated with anecdotes from experience with the NAVY, ARPA, NASA and General Motors.

1:03PM V3.00004 The History of Science and Technology at Bell Labs. DAVID BISHOP, Bell Labs, LGS, Alcatel-Lucent — Over the last 80 years, Bell Labs has been one of the most scientifically and technologically productive research labs in the world. Inventions such as the transistor, laser, cell phone, solar cell, negative feedback amplifier, communications satellite and many others were made there. Scientific breakthroughs such as discovery of the Big Bang, the wave nature of the electron, electron localization and the fractional quantum hall effect were also made there making Bell Labs almost unique in terms of large impacts in both science and technology. In my talk, I will discuss the history of the lab, talk about the present and give some suggestions for how I see it evolving into the future.

1:39PM V3.00005 50 Years of “Scaling” Jack Kilby’s Invention. ROBERT DOERING, Texas Instruments — This year is the 50th anniversary of Jack Kilby’s 1958 invention of the integrated circuit (IC), for which he won the 2000 Nobel Prize in Physics. Since that invention in a little yellow lab at Texas Instruments, IC components have been continuously miniaturized which has resulted in exponential improvement trends in their performance, energy efficiency, and cost per function. These improvements have created a semiconductor industry that has grown to over $250B in annual sales. The process of reducing integrated-circuit component size and associated parameters in a coordinated fashion is traditionally called “feature-size scaling.” Kilby’s original circuit had active (transistor) and passive (resistor, capacitor) components with dimensions of a few millimeters. Today, the minimum feature sizes on integrated circuits are less than 30 nanometers for patterned line widths and down to about one nanometer for film thicknesses. Thus, we have achieved five orders of magnitude in linear-dimension scaling over the past fifty years, which has resulted in about ten orders of magnitude increase in the density of IC components, a representation of “Moore’s Law.” As IC features are approaching atomic dimensions, increasing emphasis is now being given to the parallel effort of further diversifying the types of components in integrated circuits. This is called “functional scaling” and “more then Moore.” Of course, the enablers for both types of scaling have been developed at many laboratories around the world. This talk will review a few of the highlights in scaling and its applications from R&D projects at Texas Instruments.

Thursday, March 13, 2008 11:15AM - 2:15PM –
Session V4 DCMP: Electronic Excitations in Organic Molecular Crystals/Fluctuating Fronts: Beyond a Popular Mean-Field Theory  Morial Convention Center 206

11:15AM V4.00001 Photoemission study on the charge transport mechanism in pentacene thin film. KAZUYUKI SAKAMOTO, Chiba University — Organic molecules are attracting much interest to use for a variety of electronic applications. Pentacene (Pn), which is one of such molecules, has a high application potential due to its high hole mobility. The hole mobility of Pn is almost comparable to that of amorphous silicon. At low temperature, the hole transport in Pn crystal has been reported to have a band-like nature, and the band-like charge transport is expected to play a major part at room temperature as well. One of the origins of the band-like transport is the adequate overlap of the pi-orbitals of adjacent molecules, which produces orbital-derived electronic bands. It is therefore essential to have a proper understanding on the electronic band structures in order to fully comprehend the charge transport mechanism of a Pn crystal. By using angle-resolved photoelectron spectroscopy (ARPES), we have measured the dispersions of the highest occupied molecular orbital (HOMO)-derived bands of single crystal Pn monolayer films grown on substrates. Two HOMO-derived, whose band dispersion widths are larger than the values predicted by theoretical calculations, were clearly observed in the ARPES spectra. Our result indicates that the overlap of the pi-orbitals of adjacent Pn molecules is larger than what was expected from theoretical calculations, and the observed dispersions suggest that the higher binding energy HOMO-derived band mainly contributes to the band-like charge transport mechanism of a Pn crystal. By analyzing the dispersions within a simple tight-binding approximation, the obtained results lead to a hole mobility of \( \mu_{th} > 34.1 \text{ cm}^2/\text{Vs} \) at 140 K.

1This work was financially supported by the 21st-century COE Program at Chiba University and by MEXT of the Japanese Government.
11:51 AM V4.00002 Bandlike transport in organic molecular crystals revealed by subpicosecond transient photoconductivity. FRANK HEGMANN, University of Alberta — The nature of charge carrier photogeneration and transport in organic molecular crystals is not completely understood. In particular, the mechanism responsible for the observed bandlike behavior of charge carriers in these materials, where the carrier mobility increases as the temperature decreases, remains unresolved and is the focus of much research. Using typical device structures to explore intrinsic properties of charge transport in organic semiconductors is complicated by the presence of defects and the necessity to make contacts to the sample. Recently, however, ultrafast techniques that use terahertz (THz) pulses for assessing the electronic properties of materials have been developed. In particular, time-resolved THz spectroscopy allows transient photoconductivity in materials to be probed with subpicosecond time resolution, providing a sensitive non-contact tool for studying the transport of charge carriers before they are trapped at defect sites. This talk will provide an overview of how THz pulses can be used to probe the nature of conductivity and bandlike behavior in organic molecular crystals and thin films.

12:27PM V4.00003 Polarons and Coulomb interactions in organic transistors. SIMONE FRATINI, Instit Neel - CNRS — In organic Field Effet Transistors (FETs), charge carriers accumulate in a two-dimensional layer at the interface between an organic crystal and a gate dielectric. The possibility of tuning several microscopic parameters such as the carrier density, the electron-electron and electron-phonon interactions makes these devices an interesting playground for fundamental physics. Recent experiments have demonstrated that depending on the gate insulator used, the electric mobility in organic FETs can be tuned from metallic-like to insulating-like. This phenomenon can be explained in terms of the formation of small polarons, due to the remote interaction of the charge carriers with the phonons of the gate material [1]. In the devices with the highest polarizabilities, experiments performed at large gate voltages (corresponding to ~ 0.1 carriers/molecule) have revealed a further reduction of the mobility, suggesting the onset of electron-electron interactions [2]. The physics of this novel regime involving both strong electron-phonon and long-range electron-electron interactions will be discussed. If time allows, I shall briefly present how the above picture is modified when the narrow-band organic crystal is replaced by graphene —a two-dimensional sheet of carbon atoms. Although the effect is less striking in that case, the remote scattering with the substrate phonons still constitutes an important limiting factor of the mobility at room temperature, that should be addressed for the design of future graphene devices [3].

References:

1:03PM V4.00004 Particle versus density models in spark formation: X-rays from pulled fronts?. UTE EBERT, CWI Amsterdam and Eindhoven Univ. Techn. — Streamer discharges govern the early stages of sparks and lightning, of spark-like phenomena in water, oil, and semiconductors, in industrial corona reactors, or in gigantic sprite discharges above thunderclouds [1,2]. Thunderstorms recently have been found to emit terrestrial gamma-ray flashes or X-rays towards satellites and towards the ground. These emissions might be explained by particle models of “pulled” streamer ionization fronts. In general, the growing discharge channel has an inner structure with multiple scales [1-3]. While the largest part of this channel can be treated in a density approximation for the electrons and ions, the dynamics of the ionization front is that of a pulled front; it is determined in the leading edge where the density approach eventually breaks down. We therefore investigate a realistic MC particle model for the motion of single electrons in a discharge in pure nitrogen. The particle model not only incorporates particle fluctuations, but also shows that the electron energies are systematically larger in the leading edge of the front than in the corresponding density model, and that the ionization level behind the front is higher as well, while the front velocity hardly changes [3]. These effects increase with increasing applied electric field and might actually cause the recently observed X-ray emission from lightning through rare very energetic runaway electrons in the tail of the distribution. Comparing the leading edge of the particle front with a linear particle avalanche, the avalanche shows the same mean density gradient and energy overshoot in its leading edge as the nonlinear front; hence the pulled front concept in this sense applies to discrete particle models as well [3]. This gives a key to understanding the above effects through analytical approximations and to develop efficient numerical methods coupling particle and density models in space.

References:

1:39PM V4.00005 Fluctuation Effects on Propagating Waves of Self-Assembly in Organosilane Monolayers. JACK DOUGLAS, NIST — Wavefronts associated with reaction–diffusion and self-assembly processes are ubiquitous in the natural world. For example, propagating fronts arise in crystallization and other diverse thermodynamic ordering processes, in polymerization fronts involved in cell movement and division, as well as in the competitive social interactions and population dynamics of animals at much larger scales. Although it is often claimed that self-sustaining or autocatalytic front propagation is well described by mean-field “reaction– diffusion” or “phase field” ordering models, it has recently become appreciated from simulations and theoretical arguments that fluctuation effects in lower spatial dimensions can lead to appreciable deviations from the classical mean-field theory (MFT) of this type of front propagation. The present work explores these fluctuation effects in a real physical system. In particular, we consider a high-resolution near-edge x-ray absorption fine structure spectroscopy (NEXAFS) study of the spontaneous frontal self-assembly of organosilane (OS) molecules into self-assembled monolayer (SAM) surface-energy gradients on oxidized silicon wafers. We find that these layers organize from the wafer edge as propagating wavefronts having well defined velocities. In accordance with two-dimensional simulations of this type of front propagation that take fluctuation effects into account, we find that the interface widths w(t) of these SAM self-assembly fronts exhibit a power-law broadening of in time w(t) ~ t^0.5, rather than the constant width predicted by MFT. Moreover, the observed exponential volumes accord rather well with previous simulation and theoretical estimates. These observations have significant implications for diverse types of ordering fronts that occur under confinement conditions in biological or materials-processing contexts.

Thursday, March 13, 2008 11:15AM - 2:15PM —
Session V5 FPS FGSA: Panel Discussion: Lessons Learned from Katrina: How to Prepare a Department for Catastrophic Events Morial Convention Center R01
stability of the faculty.

The university has asked every department and unit to prepare emergency preparedness plans. Each department has been asked to collect e-mail addresses and begun coordinating with faculty. Xavier created a web page with advice for students, and the chair of the department created a separate blog with contact information for students. The early lack of a clear method of communication made worse the confusion and dismay among the faculty on such issues as when the university would reopen, whether the faculty would be retained, whether they should seek temporary (or permanent) employment elsewhere, etc. With the vision and determination of President Dr. Francis, Xavier was able to reopen the university in January and ran a full academic year from January through August. Since Katrina, the university has asked every department and unit to prepare emergency preparedness plans. Each department has been asked to collect e-mail addresses (non-Xavier), cell phone numbers and out of town contact information. The University also established an emergency website to communicate. All faculty have been asked to prepare to teach classes electronically via Black board or the web. Questions remain about the longer term issues of the size and stability of the faculty.

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11:15AM V5.00001 Lessons Learnt From Hurricane Katrina. , MURTY AKUNDI, Xavier University of Louisiana — Hurricane Katrina devastated New Orleans and its suburbs on Monday August 29th, 2005. The previous Friday morning, August 26, the National Hurricane Center indicated that Katrina was a Category One Hurricane, which was expected to hit Florida. By Friday afternoon, it had changed its course, and neither the city nor Xavier University was prepared for this unexpected turn in the hurricane’s path. The university had 6 to 7 ft of water in every building and Xavier was closed for four months. Students and university personnel that were unable to evacuate were trapped on campus and transportation out of the city became a logistical nightmare. Email and all electronic systems were unavailable for at least a month, and all cell phones with a 504 area code stopped working. For the Department, the most immediate problem was locating faculty and students. Xavier created a list of faculty and their new email addresses and began coordinating with faculty. Xavier created a web page with advice for students, and the chair of the department created a separate blog with contact information for students. The early lack of a clear method of communication made worse the confusion and dismay among the faculty on such issues as when the university would reopen, whether the faculty would be retained, whether they should seek temporary (or permanent) employment elsewhere, etc. With the vision and determination of President Dr. Francis, Xavier was able to reopen the university in January and ran a full academic year from January through August. Since Katrina, the university has asked every department and unit to prepare emergency preparedness plans. Each department has been asked to collect e-mail addresses (non-Xavier), cell phone numbers and out of town contact information. The University also established an emergency website to communicate. All faculty have been asked to prepare to teach classes electronically via Black board or the web. Questions remain about the longer term issues of the size and stability of the faculty.

11:30AM V5.00002 TBD , SHIRLEY LASKA, University of New Orleans — This abstract has not been submitted.

11:45AM V5.00003 Hurricane Katrina at Tulane. , JIM MCCUIRGE, Tulane University — After hurricane Katrina struck New Orleans on August 29, 2005, Tulane University closed for the fall semester. Buildings on campus were closed and armed guards were hired to protect the campus. Faculty members were not allowed access to their offices and laboratories, except for exceptional cases when a Dean went with them. Many faculty members took their research groups to other universities accepting much welcomed invitations from colleagues. Undergraduates went to other colleges and universities, which accepted the without cost and a promise not to recruit them. The university email system went down for months. Collecting information on the welfare of faculty and students was difficult. The university was run from Houston by a small handful of senior administrators. Setting up the schedule of classes for the spring 2006 semester was done without records. Most faculty returned to New Orleans after several weeks. 80% of the city was flooded. Small trailers were provided. Some lived in the FEMA trailers for two years or more. When Tulane reopened, a wide reaching Renewal Plan, worked out by the upper administration, was implemented. A new emergency preparedness plan was also developed and put in place.

12:00PM V5.00004 , G. GREG SEAB, University of New Orleans — No abstract available.

12:15PM V5.00005 Academic environment and dynamics in response to extreme events: Theory and Practice (Katrina Lessons)1, NATALIA SIDOROVSKAIA, Department of Physics, University of Louisiana at Lafayette — The possibility of a catastrophic event requires the department as a unit and the university as an organization to devise a comprehensive emergency response plan to minimize the impact and shorten the recovery stage. Does the academic organizational structure and environment possess key features for the possibility of successful response to extreme events? The post Hurricane Katrina experience of Louisiana universities offers data to address this theoretical question. It also emphasizes that the mitigation plan should include two aspects: preparing/protection a university for/during a catastrophic event and assisting other academic institutions experiencing an extreme event. Short-term and long-term statistics and other data pertain to the interaction of the University of Louisiana at Lafayette (as an assistance unit) with the universities in New Orleans (units in distress), including the dynamics of student population, faculty influx, course adjustments, and response and recovery actions are presented. An attempt is made to categorize the losses and to assess the recovery quality and time. Faculty and institutional administration interviews are summarized to assist in developing future proactive response plans. UL Lafayette and UNO research capabilities and intellectual resources for developing complex models simulating the multi-variable effects of catastrophic events and providing adaptability in the decision-making process are investigated.

1This work was done in collaboration with George E. Ioup and Juliette W. Ioup (Department of Physics, University of New Orleans).

12:30PM V5.00006 Hosting a Katrina Evacuee. , DAVID HOAGLAND, Polymer Sci. and Eng. Dept., Univ. of Massachusetts Amherst — No individual or institution anticipated the impact on the academic research community of hurricane Katrina. When Tulane physicist Wayne Reed asked me to host his research group just a day or two after the disaster, with no authorization or understanding of the commitment, I agreed immediately and then pondered implications. Fortunately, colleagues helped in making the commitment real, only the bureaucracy of my public university posing small hindrances. Industry was remarkably generous in providing Reed with significant “loaner” equipment, and amazingly, a suite of custom Reed experiments was running within weeks. At the end, the most productive collaborations for Reed seemed not to have been with my group, with its similar research, but to other groups at my institution, particularly the synthetic chemists, who gained access to methods previously unique to Tulane while offering samples previously unique to UMass. Quickly designed projects exploiting this match turned out remarkably productive. Although begun with trepidation, hosting of Reed had huge positive benefits to me and UMass, and I believe, also to Reed and Tulane. Some key lessons for the future: (i) industry has capacity and willingness to help academic research during disruption (ii) commitment of a host institution must be immediate, without a wait for formal approvals or arrangement of special funding – delay leads only to discouragement, (iii) continuing academic progress of displaced students must come first, and (iv) intellectual synergy rather than overlap should be the basis for seeking a host. Lastly, NSF or other funding agency should consider a program directly addressing the research needs of unexpectedly disrupted academic scientists, and most particularly, graduate students who face greatly extended studies.

12:45PM V5.00007 Panel Discussion —
**11:15AM V7.00001 Building the Vertebrate Spine**, OLIVIER POURQUÉ, Howard Hughes Medical Institute and Stowers Institute for Medical Research — The vertebrate body can be subdivided along the antero-posterior (AP) axis into repeated structures called segments. This periodic pattern is established during embryogenesis by the somitogenesis process. Somites are generated in a rhythmic fashion from the paraxial mesoderm and subsequently differentiate to give rise to the vertebrae and skeletal muscles of the body. Somite formation involves an oscillator-the segmentation clock-whose periodic signal is converted into the periodic array of somite boundaries. This clock drives the dynamic expression of cyclic genes in the presomitic mesoderm and requires Notch and Wnt signaling. Microarray studies of the mouse presomitic mesoderm transcriptome reveal that the segmentation clock drives the periodic expression of a large network of cyclic genes involved in cell signaling. Mutually exclusive activation of the Notch/FGF and Wnt pathways during each cycle suggests that coordinated regulation of these three pathways underlies the clock oscillator. In humans, mutations in the genes associated to the function of this oscillator such as Dll3 or Lunatic Fringe result in abnormal segmentation of the vertebral column such as those seen in congenital scoliosis. Whereas the segmentation clock is thought to set the pace of vertebrate segmentation, the translation of this pulsation into the reiterated arrangement of segment boundaries along the AP axis involves dynamic gradients of FGF and Wnt signaling. The FGF signaling gradient is established based on an unusual mechanism involving mRNA decay which provides an efficient means to couple the spatio-temporal activation of segmentation to the posterior elongation of the embryo. Another striking aspect of somite production is the strict binary symmetry of the process. Retinoic acid was shown to control aspects of this coordination by buffering destabilizing effects from the embryonic left-right machinery. Defects in this embryonic program controlling vertebral symmetry might lead to scoliosis in humans. Finally, the subsequent regional differentiation of the precursors of the vertebrae is controlled by Hox genes, whose collinear expression controls both gastrulation of somite precursors and their subsequent patterning into region-specific types of structures. Therefore somite development provides an outstanding paradigm to study patterning and differentiation in vertebrate embryos.

**11:51AM V7.00002 Modelling Ultradian Oscillations and Segmentation**, MOGENS JENSEN, Niels Bohr Institute — We model ultradian oscillations in four different eucaryotic systems: Hes1, p53-mdm2, NF-kB and Wnt-Notch. In each of the systems we identify the feed-back loops for the genetic regulations. Oscillations are possible when time delays are present, either by directly introducing a delay, by many steps in the loops or by saturated degradation. The oscillations are important for apoptosis and control of inflammation. The Wnt-Notch system is essential in embryo segmentation and we introduce a model in which the Wnt oscillates by itself but drives the Notch cycle out of phase with the Wnt cycle, in good agreement with experimental observations.

**12:27PM V7.00003 Spatial Patterns of Recurred Sensory Organs in Drosophila**, GEMUNU GUNARATNE, University of Houston — The fruit fly Drosophila is one of the most intensely studied models of development. A subset of nominally identical cells on the anterior wing of Drosophila begins to differentiate at puparium formation, each developing a sensory organ. In wild type flies, every fifth cell becomes such a sensory organ. Recent studies on mutant flies have shown that the transcription factor Senseless and the micro RNA mIR-9a play significant roles in the choice of bristle density and the regularity of their arrangement. We propose that this cell differentiation is due to a Turing-type bifurcation whereby periodic concentration gradients emerge spontaneously from a uniform background. A paradigmatic model with intra-cellular networks and lateral activation and inhibition between neighboring cells (for example, through the Notch signaling pathway) is shown to generate the observed arrangements of sensory organs. The theory makes several experimentally verifiable predictions. For example, we propose methods to create mutant flies with systematically increasing numbers of ectopic bristles. In our theory, post-transcriptional regulatory action of the micro RNA occurs through the choice of stable solutions of the network.

**1:03PM V7.00004 Similarities and differences in the p53-mdm2 and NF-kB feedback loops**, SANDEEP KRISHNA, Niels Bohr Institute, University of Copenhagen — Ultradian oscillations in the p53 and NF-kB signalling systems are produced using similar mechanisms: a negative feedback loop combined with an effective time delay. However, seemingly small differences in the molecular implementation of this mechanism mean that the NF-kB system is in equilibrium in the resting state, while the p53 system is far from equilibrium. I will discuss how this affects the dynamical response of the systems. In particular, I will argue that the nonequilibrium driving makes the p53 system respond much faster to external stimuli than the NF-kB system. The interesting question then is whether this makes sense physiologically, and is consistent with the fact that p53 triggers cell-cycle arrest and apoptosis, while NF-kB triggers the immune response.

**1:39PM V7.00005 Dynamic Changes in microRNAs may Regulate Robustness of Wnt/Notch Signaling**, FREETHI GUNARATNE, University of Houston — The mechanisms by which highly reproducible patterns are formed during embryonic development and organismal evolution despite stochasticity at the single cell level is one of the remaining mysteries in Biology. It has been proposed that a hidden layer of regulation formed through the interaction of microRNAs with protein coding gene networks maybe responsible. Recently developed next generation sequencing technologies afford an unprecedented opportunity to uncover novel aspects of microRNA function and evolution. We find extensive heterogeneity in sequences that correspond to mmu-let-7 (targets Wnt1) and mmu-miR-191 (targets Notch1). Approximately 20% of let-7 and miR-191 have undergone modifications to increase stability and binding to the Wnt1 and Notch1 targets and are likely to be destroyed. In contrast, 80% bind the targets with imperfect complementarity and lower stability and are likely to be sequestered and prevented from forming protein. We propose that these two species together form a highly fluid system that is able to absorb stochastic perturbations in gene expression. A gene that goes on to be translated into functional protein therefore must escape both buffers by significantly high expression.

**Thursday, March 13, 2008 11:15AM - 2:03PM**

**Session V8 DFD: Liquid Crystals I: Structure and Defects**

**11:15AM V8.00001 Effect of Concentration Variations on the Interaction of a Sm-A Liquid Crystal and a Nanoparticle**, LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, LYNN K. KURIHARA, Navy Research Lab, Washington, DC, RAHINA S. RABIU, University of Maryland and Norfolk State University — We have observed the evolution of the interaction between a Sm-A Liquid Crystal (8CB) and a nanoparticle as the concentration of the nanoparticle is reduced from 30% wt to 0.1%wt. We have observed that a linear structure is observed as the concentration of the particle falls below 15% wt. There is a difference between the functionalization compounds as observed in the study of the 30% wt mixtures. In addition, we have observed that the influence of the nanoparticle in the ordering or disordering of the liquid crystal can be quantified through the integrated intensity of the x-ray signal.

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1 We acknowledge NSF-DMR grant number 0520471 for partial support of this work.
2 REU student
11:27 AM V8.00002 Simulating defect structures in nematic liquid crystal shells1,2, LENA LOPATINA, ANDREW KONYA, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ, ALEX TRAVESSE, Dept of Physics and Astronomy, Iowa State Univ — Recent theoretical and experimental studies have investigated nematic liquid crystals confined to a shell between two spheres. When the shell is very thin, the structure provides an experimental realization of nematic order and defects in a 2D curved geometry. As the shell becomes thicker, the behavior crosses over to a 3D liquid crystal, with different types of defects. To study this dimensional crossover, we perform simulations of nematic order in a shell. For these simulations, we use a disordered lattice, or mesh, constructed through random sequential adsorption on the inner surface, the outer surface, and within the bulk of the shell, with a nematic director on each site of the mesh. By minimizing the energy, we determine the nematic texture as a function of the radii and thickness of the shell, and as a function of the off-center displacement of the inner sphere. The results show a crossover between half-charged vortex line defects for thin shells and boojum pairs for thicker shells, and demonstrate a new equilibrium state with two vortex lines and one boojum pair. They also show a complex evolution of the structures and energy as the inner sphere moves off-center.

1Supported by NSF DMR-0605889 and DMR-0426597 and by ICAM.

11:39 AM V8.00003 String defects in smectic-C monolayers and hybrid nematic films1,2, FANGFU YE, ZHAO LU, LENAPATINA, JONATHAN SELINGER, Liquid Crystal Institute, Kent State Univ, ALEX TRAVESSE, Dept of Physics and Astronomy, Iowa State Univ — Defects are important in determining the structure and statistical mechanics of liquid crystals. In this project, we study the structure of topological defects in smectic-C monolayers and hybrid nematic films. When subjected to boundary conditions requiring a total topological charge of +1, the classical xy model in a flat disk geometry has a ground state of a single vortex of charge +1. By comparison, perfect nematics with directors in the same 2D geometry have two +1/2 vortices repelling each other. We show that slightly tilting directors out of the plane to form a smectic-C monolayer yields two +1/2 vortices bound together by a domain wall, which we call a string defect. We also develop a model easily testable in experiments, in which a thick nematic film is constrained in a cell with weak homeotopic anchoring on one surface and strong planar anchoring on the other surface. For this model, we derive the phase diagram and investigate how the length of string defects changes with the thickness of the cell. We further present numerical simulations of the nematic director in the hybrid film.

1Supported by NSF DMR-0605889 and DMR-0426597 and by ICAM.

2Currently at College of Veterinary Medicine, Cornell Univ.

11:51 AM V8.00004 Coherent anti-Stokes Raman scattering polarized microscopy of 3D director structures in liquid crystals1,2, IVAN SMALYUKH, University of Colorado at Boulder, ALEXANDER KACHYNSKI, ANDREY KUZMIN, LONAS PRASAD, The State University of New York at Buffalo — We demonstrate labeling-free three-dimensional imaging of director structures in liquid crystals using coherent anti-Stokes Raman scattering (CARS) polarized microscopy [1]. Spatial mapping of the structures is based on the strong sensitivity of a polarized CARS signal to the orientation of selected chemical bonds of anisotropic molecules in liquid crystals. As an example, we study director structures in cholesteric, nematic, and smectic materials. We demonstrate that the CARS images of molecular orientation patterns are consistent with the structure models and with the respective computer-simulated CARS textures.


1Research was supported by the Directorate of Chemistry and Life Sciences of Air Force Office of Scientific Research, by International Institute for Complex Adaptive Matter, and the National Science Foundation, Grant DMR #0645461.

12:03 PM V8.00005 Light Scattering Study of Biaxiality in Nematic Liquid Crystal Tetrapodes, KRISHNA NEUPANE, SHINWOONG KANG, SUNIL SHARMA, D. CARNEY, T. MEYER, GEORGE H. MEHL, DAVID W. ALLENDER, SATYENDRA KUMAR, SAMUEL SPRUNT, Department of Physics, Kent State University — We have performed dynamic light scattering studies on thermotropic liquid crystalline tetrapodes [1], which reportedly exhibit a uniaxial to biaxial nematic phase transition. Our results [2] support the existence of the biaxial nematic phase in tetrapodes. The uni- to biaxial transition is found to be weakly first-order in a 4-ring tetrapode and second-order in a 3-ring tetrapode, while the isotropic to uniaxial nematic transition is weakly first order in both materials. The temperature dependence of the relaxation rates of the biaxial order parameter modes, and of the intensity associated with biaxial director fluctuations, is explained by a Landau-deGennes model of the free energy.


12:15 PM V8.00006 Effects of dielectric relaxation on the director dynamics of uniaxial nematic liquid crystals1,2, MINGXIA GU, YE YIN, SERGUJ V. SHYANOVSII, OLEG D. LAVENTOVICEH, Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, Ohio 44242, USA — We derive the reorienting dielectric torque acting on the director, considering the frequency dependence of the dielectric tensor. The model takes account into the effects of multiple relaxations in both parallel and perpendicular components of the dielectric tensor and predicts the “dielectric memory effect” (DME), i.e., dependence of the dielectric torque on both the “present” and “past” values of the electric field and the director. In a sharply rising electric field, the DME slows down director reorientation for the materials whose dielectric anisotropy is positive at low frequencies, but speeds up the response for the dielectrically negative materials. We also demonstrate, both theoretically and experimentally that an induced “memory” polarization leads to a dielectric torque in the switch-off phase which has an opposite sign to that of the LC's dielectric anisotropy, when a thick nematic film is constrained in a cell with weak homeotopic anchoring on one surface and strong planar anchoring on the other surface. For this model, we derive the phase diagram and investigate how the length of string defects changes with the thickness of the cell. We further present numerical simulations of the nematic director in the hybrid film.

1Supported by DOE Grant No. DE-FG02-06ER 4631.

12:27 PM V8.00007 Condensation of lyotropic chromonic liquid crystals by additives1,2, LUANA TORTORA, H.-S. PARK, Liquid Crystal Institute, Kent State University, Kent, OH 44242, S.-W. KANG, Department of Physics, Kent State University, Kent, OH 44242, S. KUMAR, Department of Physics, Kent State University, Kent, OH 44242 and DMR NSF, K.V. KAZNATCHEEV, Canadian Light Source, SK S7N 0X4, Canada, O.D. LAVRENTOVICEH, Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH 44242 — Lyotropic chromonic liquid crystals (LCLCs) are formed by molecules with rigid polyaromatic cores and ionic groups at the periphery that aggregate in water. Condensation of LCLCs can be driven by polyanions, organic salt and neutral polymers. At a suitable concentration of additives, a nematic LCLC demixes into a coexisting isotropic phase and a condensed phase with birefringence higher than that in the original N. By employing synchrotron X-ray scattering we demonstrate the formation of a columnar hexagonal (C) phase. Scanning transmission X-ray microscopy, LC PolScope and fluorescent confocal microscopy allow us to map the relative concentration of components in the condensed and isotropic regions. Both electrostatic and entropy effects contribute to the condensation.

1Supported by NSF DMR 0504516, DMR 076290, AFOSR MURI FA9550-06-1-0337, Samsung Electronics Corp.
12:39PM V8.00008 Interactions in the NOBOW and 8CB Mixtures1. DONG CHEN, CHENHUI ZHU, NOEL CLARK, Department of Physics, University of Colorado, Boulder — Mixtures of a bent-core mesogen (NOBOW) and a calamitic mesogen (8CB) are studied using X-ray diffraction (XRD), polarized light microscopy and freeze fracture electron microscopy (FFEM). XRD shows that as the 8CB concentration increases, the transition temperature of Iso-B4 decreases and the correlation length of NOBOW B4 decreases while the correlation length of 8CB SmA increases. Polarized light microscopy reveals that the mixtures have larger chiral domains than pure NOBOW and when the phase of 8CB changes to SmA, they show the same boundary as the chiral domains. FFEM images show more details on the structure of the mixtures. Along with the experiments, we will present theoretical studies on the interactions in the NOBOW and 8CB mixtures.

1This work is supported by NSF MRSEC Grant DMR-0213918

12:51PM V8.00009 Effect of Solvent Concentration on the Liquid Crystal Phase Transitions of Octylocyanobiphenyl-Hexane Mixtures, KRISHNA SIGDEL, GERMANO IANNACCIONE, WPI — The effect of a non-mesogenic, low-molecular-weight, solvent on the phases of a liquid crystal can be profound. High-resolution ac-calorimetry has been carried out on the isotropic (I-N) and the nematic to smectic-A (N-SmA) phase transitions of the liquid crystal octylocyanobiphenyl (8CB) as a function of hexane concentration. Temperature scans were performed above and below these transition temperatures for all samples. Six 8CB-hexane samples were studied having molar concentrations of 0.017 (0.5% by mass), 0.033 (1%), 0.063 (2%), 0.078 (2.5%), 0.092 (3%) and 0.119 (4%) of hexane. Upon increasing dilution of 8CB by the linear form of hexane, the transition temperatures shift lower while the order of both transitions evolves. These effects may be the consequence of the weakening of the liquid crystal molecular interactions due to the presence of the solvent.

1:03PM V8.00010 Landau potential of polymer stabilized ferroelectric liquid crystals, PAUL ARCHER, INGO DIERKING, The University of Manchester — Polymer stabilized liquid crystals (PSLC) [1] consist of a relatively low concentration of a photo-polymerized monomer (typically less than 10%wt) which is phase separated from the continuous liquid crystal medium. For the case of a polymer stabilized ferroelectric liquid crystal, photo-polymerized in the SmA* phase, the network forms parallel to the smectic layer normal. This results in an elastic coupling between the polymer network and the liquid crystal which alters the characteristics of the SmA* to SmC* phase transition. The generalized model of ferroelectric liquid crystals has been modified to encompass this additional interaction through a polymer coupling coefficient. Analysis of experimental tilt angle and polarization data allows the determination of the polymer coupling coefficient and hence the full Landau potential. Results will be shown and discussed for varying polymer concentration.


1:15PM V8.00011 Varying the optical properties of cholesteric liquid crystals, SABRINA RELAIX, MICHELE MOREIRA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU, MICHEL MITOV, CEMES/CNRS — Cholesteric Liquid Crystals (CLCs) are of particular interest as they form self-assembled photonic band gap (PBG) structures - a macroscopic helical structure, leading to a selective reflection of light - which can be easily tuned by external fields. As PBG materials, CLCs have been used as mirrorless lasers with low lasing thresholds since the density of photon states is suppressed in the reflection band and is enhanced at its edges [1]. The modification of the cholesteric organization – either by the introduction of a pitch gradient across the cell or by the incorporation of nanoparticles in the medium – has direct consequences on the PBG and hence the reflected intensity [2,3]. In this presentation, I will describe the variations in the optical properties of CLC caused by these modifications and will discuss possible applications, such as tuning the CLC laser wavelength or adjusting the laser threshold.


1:27PM V8.00012 Three-dimensional imaging of chemical bond orientation in liquid crystals by coherent anti-Stokes Raman scattering microscopy,1. OLEG D. LAVRETOVICH, HEUNG-SHIK PARK, Liquid Crystal Institute and Chemical Physics Program, Kent State University, Kent, OH 44242, BRIAN G. SAAR, X. SUNNEY XIE, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138 — Coherent anti-Stokes Raman scattering (CARS) microscopy is used to provide three-dimensional chemical maps of liquid crystalline (LC) samples without the use of external labels. CARS is a polarization-sensitive optical imaging technique that derives contrast from Raman-active molecular vibrations in the sample. Compared to other three-dimensional imaging techniques, CARS offers the most rapid chemical characterization available without the use of external dyes or contrast agents. Examples that illustrate the applicability of CARS microscopy to LCs include textures and defects in nematic and smectic LC, electric Frederiks transition.

1Supported by NSF DMR 0504516, DBI-0649892, Keck Foundation, AFOSR MURI FA9550-06-1-0337

1:39PM V8.00013 Low electric field induced phase transition of the B1 bent-core liquid crystal phase to a switching phase, J. KIRCHHOFF, L.S. HIRST, Florida State University — Liquid crystal materials that have ferroelectric and antiferroelectric phases are useful in applications due to their switching properties. The B1 bent-core liquid crystal phase is a columnar phase that does not exhibit switching. A transition from the B1 liquid crystal phase to a switching phase has been seen at an electric field of 10 V/μm, which is much lower than previously seen fields of greater than 25 V/μm [1]. This transition is irreversible upon reduction of the applied field and switching continues almost threshold-less down to an applied field of 40 mV/μm, which has not been previously reported. Any amount of a chiral rod-like dopant increases the field required to transition from the B1 to the switching phase, and the transition becomes reversible with the switching phase relaxing back to the B1 phase after a decrease in the electric field. A small concentration of the rod-like dopant also induces a change from the B1 phase to a new liquid crystal phase. These effects were studied using polarized optical microscopy, calorimetry (DSC), and x-ray measurements.


1:51PM V8.00014 Evidence of Broken Reciprocity in Chiral Liquid Crystals, MICHELE MOREIRA, NITHYA VENKATARAMAN, BAHMAN TAHERI, PETER PALFFY-MUHORAY, Liquid Crystal Institute, KSU — Reciprocity in light scattering is predicated on bounded scattering media with symmetric and linear permittivity, conductivity and permeability. Due to their anisotropy and chirality, cholesteric liquid crystal form periodic dielectric structures. If the periodicity is comparable to the wavelength of light, these phases are self-assembled photonic band gap structures. There appear in the permittivity odd powers of the wave vector resulting from nonlocality and broken inversion symmetry. Evidence of non-reciprocity has been found in optically active crystals by Bennett [1] and in stacks of cholesteric and nematic liquid crystal cells by Takezoe [2]. We present experimental data showing broken reciprocity in transmittance and reflectance in cholesteric cells with different pitches having overlapping but distinct reflection bands. We explain our results in terms of simple analytic descriptions of material properties and propagating modes.

Under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes. Retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes. Retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed.

KATHIE E. NEWMAN, Physics, U. of Notre Dame — A new algorithmic method is discussed, Non-Adiabatic Path Sampling (NAPS), which combines features of transition path sampling (TPS) and molecular dynamics with quantum transitions (MDQT). The goal is to ultimately address problems which involve excited and coupled electronic states, as well as large systems and long timescales (e.g., semiconductor photocatalysis). TPS focuses specifically on trajectories that take the system from reactants to products, which allows the study of chemically producible processes dominated by rare but important events whose timescales are outside the range of direct simulation. In the MDQT algorithm, the nuclear dynamics of the system do not occur on a single Born-Oppenheimer potential energy surface, but rather may involve non-adiabatic transitions between many coupled electronic states. The NAPS algorithm uses the statistical framework of TPS to analyze MDQT trajectories, using the advantages of each method to get results for otherwise inaccessible systems. The algorithm is tested on a simple model of proton transfer. A quantum-mechanical proton in a double-well quartic potential bi-linearly coupled to a thermal bath of classical harmonic oscillators. Results from the model are compared to numerically exact results available in the literature.

ZHANG, KARSTEN REUTER, Fritz-Haber-Institut der Max-Planck Gesellschaft — With respect to oxidation catalysis or oxide formation, surface defects like steps, kinks, or vacancies are widely believed to play a decisive role, e.g., in form of active sites or as nucleation centers. Despite this suggested importance, first-principles investigations qualifying this role for gas-phase conditions that are representative of these applications are scarce. This is mostly due to the limitations of electronic-structure calculations in tackling the large system sizes and huge configuration spaces involved. We overcome these limitations with a first-principles statistical mechanics approach coupling density-functional theory (DFT) calculations with grand-canonical Monte Carlo simulations, and apply it to obtain the phase diagram of on-surface O adsorption at a (111) step on a Pd(100) surface. The link between the electronic and mesoscopic techniques is achieved by a lattice-gas Hamiltonian expansion, in which we parameterize the lateral interactions affected by the step from DFT calculations at a Pd(111) vicinal surface, and all remaining lateral interactions from calculations at Pd(100). For a wide range of O gas-phase conditions we find the (111) step to be decorated by a characteristic zig-zag structure. Intriguingly, this structure prevails even up to the elevated temperatures characteristic for catalytic combustion reactions, where only small amounts of disordered oxygen remain at the Pd(100) surface.

VASILY BULATOV, Lawrence Livermore National Lab — The key challenge in simulations of irradiated materials is that of time scale. Typically, atomistic simulations extend to less than one nanosecond whereas kinetic Monte Carlo (kMC) simulations struggle to reach hours of simulated irradiation. Based on a time-dependent Green’s function formalism, our new kMC algorithm extends the simulated time horizon from minutes to tens and hundreds of years while retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes.

1 This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. (UCRL-ABS-236713).

11:39AM V9.00003 First-passage Monte Carlo for materials under irradiation1, ALEKSANDAR DONEV, VASILY BULATOV, Lawrence Livermore National Lab — The key challenge in simulations of irradiated materials is that of time scale. Typically, atomistic simulations extend to less than one nanosecond whereas kinetic Monte Carlo (kMC) simulations struggle to reach hours of simulated irradiation. Based on a time-dependent Green’s function formalism, our new kMC algorithm extends the simulated time horizon from minutes to tens and hundreds of years while retaining uncompromising accuracy. This presents an exciting opportunity to extrapolate, through accurate numerical simulations, the material behavior observed under the short and violent irradiation exposures used in the accelerated material tests, to the much longer reactor material lifetimes.
12:27PM V9.00007 Solidifying semiconductor nanocrystals from melts: Molecular dynamics simulations. TIANSHU LI, DAVIDE DONADIO, GIULIA GALLI, Department of Chemistry, University of California, Davis — Understanding the nucleation of semiconductor nanocrystals is of fundamental importance in the field of nanoscience. In this study we employ classical molecular dynamics simulations to explore the crystallization of Si nanocrystals from the melt. We focus on the differences between homogeneous and heterogeneous nucleations, where the heterogeneous case is investigated by simulating a liquid slab. In particular, we use the recently developed forward fluxing method [R.J. Allen, D. Frenkel, and P.R. ten Wolde, JCP 124 024102(2006)] to model the evolution of nucleation processes from melts and to compute nucleation rates. We demonstrate that free surfaces act as catalytic nucleation sites by significantly promoting the formation of solid-like small clusters. The presence of solid-like clusters in proximity of the surfaces is found to occur at temperature higher than those at which solid seed nucleation occurs in bulk liquids, highlighting the important role of heterogeneous nucleation under low-under-cooling conditions.

12:39PM V9.00008 Ab-Initio Density Functional Calculation of Interatomic Potentials for Large-scale Atomistic Material Simulations. G.L. ZHAO, Department of Physics and High Performance Computing Laboratory, Southern University and A&M College, Baton Rouge, Louisiana 70813, S. YANG, Department of Physics, Southern University and A&M College — We propose a new method to calculate interatomic potentials, utilizing an ab-initio density functional formalism. The calculated interatomic potentials can be used for large scale atomistic material simulations and predictions. We benchmark the method for the case of copper. We utilized the ab-initio interatomic potential to calculate various properties of transition metal copper, including the lattice constant, the bulk modulus, thermal expansion coefficient, monovacancy formation energy, and phonon frequencies. The calculated results agree very well with experimental values. We further calculated the properties of BCC Cu, utilizing the interatomic potential derived from the electronic structure calculations of FCC Cu, to demonstrate the predictive capabilities of the interatomic potential. The predicted properties of BCC Cu agree very well with experimental and ab-initio density functional results. Part of the work was performed during the stay of G. L. Zhao at Princeton University. The authors gratefully acknowledge the financial support of the National Science Foundation (Award No. 0508245).

12:51PM V9.00009 A New Look at the Evaluation of Embedded Atom Potential Models.1 JAMES N. GLOSII, KYLE J. CAPSERSEN, DAVID F. RICHARDS, ROBERT E. RUDD, FRED H. STREITZ, Lawrence Livermore National Laboratory — The embedded atom method (EAM) potentials have been used extensively since introduced by Daw and Baskes in the mid 1980’s due to their simple incorporation of many-body effects that are missed by simple pair potentials. The computational cost of the inclusion of this additional physics has traditionally been a second pass over the pair data. We will report on an implementation of the EAM model within a molecular dynamics algorithm (MD) that does not require this second pass, substantially reducing the computer time and memory required for evaluation of the potential. The second pass is avoided by using a forward extrapolation in time of the density derivative of the embedding function $dF(\rho(t))/d\rho$. The error in this approximation is controllable and consistent with the error introduced by the finite time step numerical integrators used in the MD.

1:03PM V9.00010 Electronic structure from Maximum Entropy optimization: Applications to band energy and electronic force computation1, HIRO SHIMOMA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — We apply a new entropy optimization scheme to study the electronic density of states for complex disordered materials from a knowledge of spectral moments. We employ the Shannon entropy functional in our work and maximize it subject to the moment constraints to construct the spectral distribution of large Hamiltonian matrix[1]. We illustrate the efficiency and the usefulness of the method by reconstructing a number of exact functions, which are difficult to reproduce by other function reconstruction techniques. The local and global convergence properties of the resulting distribution is studied and the band energy and Fermi level are computed with a high degree of precision. An extension of this method to calculate electronic forces is presented for the purpose of using in large-scale molecular dynamics simulation of materials.

1:15PM V9.00011 Lagrangian Time-Reversible Born-Oppenheimer Molecular Dynamics. ANDERS NIKLASSON, Theoretical Division Los Alamos National Laboratory — A Lagrangian generalization of time-reversible Born-Oppenheimer molecular dynamics [Niklasson et al., Phys. Rev. Lett., vol.97, 123001 (2006)] is proposed. The new formulation enables highly efficient symplectic or geometric integrations of both the nuclear and the electronic degrees of freedom that are stable and energy conserving even under incomplete self-consistency convergence. It is demonstrated how the accuracy is improved by over an order of magnitude compared to previous formulations at the same level of computational cost. The proposed Lagrangian includes extended electronic degrees of freedom as auxiliary dynamical variables in addition to the nuclear coordinates and momenta. While the nuclear degrees of freedom propagate on the Born-Oppenheimer potential energy surface, the extended auxiliary electronic degrees of freedom evolve as a harmonic oscillator centered around the adiabatic propagation of the self-consistent ground state (http://arxiv.org/abs/0711.3466).

1:27PM V9.00012 First-principles calculation combined with multicanonical simulation, YOSHIFUJI YOSHIMOTO, ISSP, University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, 2778581, Japan — To tackle statistical complexities in condensed matters such as phase transitions of atomic structures with first-principles calculations, Yoshimoto have studied the combination of first-principles calculations and multicanonical methods. By the multicanonical methods, phase space of atomic coordinates can be explored efficiently. Among phase transitions, Yoshimoto focused crystal—liquid transition because it is a basic process for material synthesis and formation of objects (casting). The talk will present his recent results: a direct proof of coexistence between the crystal—liquid transition by a kind of two-component multicanonical ensemble, a multi-order multi-thermal ensemble, with an order parameter defined with structure factors that characterize the transition, and optimization of a model interatomic potential in terms of the ensemble from an accurate one called thermodynamic downfolding of a potential. These provide a principle to project a first-principles approach on a model-based approach containing thermodynamic properties of multiple phases to a maximum of transition. The talk will cover the successful applications of the method to the transition of Si and MgO. Ref: Y. Yoshimoto, J. Chem. Phys. 125, 184103 (2006)

1:39PM V9.00013 Topological Properties of Microstructures in Nanocrystalline Materials. TAO XU, MO LI, Georgia Institute of Technology — Recent experiments show that the topological properties of microstructures in nanocrystalline materials play an important role in the mechanical properties of nanocrystalline materials. However, the fundamental structure-property relationship has not been fully understood due to the difficulties in determining and controlling the microscopic properties of nanocrystalline materials experimentally. In this study, we investigate how different topological properties affect the thermal and mechanical responses of nanocrystalline materials, including grain size distribution, surface area distribution, triple junction length distribution, grain boundary misorientation, etc. Digital microstructures with desired topological properties are generated using Inverse Monte Carlo method and are then relaxed and deformed by large-scale molecular dynamic simulation. In order to characterize the relaxed and deformed digital samples, we use a new grain boundary characterization method to accurately determine the position and thickness of each grain boundary during both relaxation and deformation. Finally, this newly developed algorithm enables us to study the correlation between topological and mechanical properties of nanocrystalline materials.
resonant soft x-ray scattering (RSXS) to answer this question for La holes can be spatially separated in an oxide heterostructure from the disordered doped layers in a way analogous to semiconductor modulation doping. We used measurements have identified a pronounced influence of the dopant atoms on microscopic properties of bulk HTS, therefore raising the question of whether the CNRS UPR5-ESPCI, Paris, France, A. GOZAR, G. LOGVENOV, I. BOZOVIC, Brookhaven National Laboratory, NY 11973, USA — Ability of grow crystalline, S. SMADICI, P. ABBAMONTE, J. LEE, S. WANG, University of Illinois at Urbana-Champaign, IL 61801, USA, C.D. CAVELLIN, Universite Paris 12 and Bi material rendered normal by severe underdoping. It may underlie recent experimental observations of the giant proximity effect between two cuprate superconductors separated by a barrier made of the same effect can undergo an enormous enhancement. We establish this novel proximity effect by a general argument as well as a numerical simulation and argue that it may underlie recent experimental observations of the giant proximity effect between two cuprate superconductors separated by a barrier made of the same material rendered normal by severe underdoping.

Supported by the Richmond F. Snyder Fund


11:15AM V10.00001 Superconducting proximity effect and Majorana fermions at the surface1, LIANG FU, CHARLES KANE, University of Pennsylvania — A strong topological insulator is an insulating material in which spin-orbit interaction inverts the band gap at an odd number of time reversed pairs of points in the Brillouin zone. These materials have topologically protected gapless spin-split surface states, whose Fermi arc is characterized by a Berry’s phase of \( \pi \). We study the proximity effect between an s-wave superconductor and the surface states of a strong topological insulator. The resulting two dimensional state resembles a spinless \( p_x + ip_y \) superconductor, but does not break time reversal symmetry. This state supports Majorana bound states at vortices. Such bound states obey non-Abelian statistics and have been studied in the context of topological quantum computing. We show that linear junctions between superconductors mediated by the topological insulator form a non chiral 1 dimensional wire for Majorana fermions, and that circuits formed from these junctions provide a method for creating, manipulating and fusing Majorana bound states.

1 Supported by NSF OCI PetaApps program ITR-HECURA 0749217

11:27AM V10.00002 Giant proximity effect in a phase-fluctuating superconductor, DOMINIC MARCHAND, LUCIAN COVACI, MONA BERCIOU, MARCEL FRANZ, Department of Physics and Astronomy, University of British Columbia — When a tunneling barrier between two superconductors is formed by a normal material that would be a superconductor in the absence of phase fluctuations, the resulting Josephson effect can undergo an enormous enhancement. We establish this novel proximity effect by a general argument as well as a numerical simulation and argue that it may underlie recent experimental observations of the giant proximity effect between two cuprate superconductors separated by a barrier made of the same material rendered normal by severe underdoping.

11:39AM V10.00003 Search for Proximity Effect in the Local Pairing Temperature of \( \text{Bi}_2\text{Sr}_2\text{Ca}_x\text{Cu}_4\text{O}_{8+x} \), COLIN PARKER, AAKASH PUSHP, KENJIRO K. GOMES, ABHAY PASUPATHY, Department of Physics, Princeton University, GENDA GU, Brookhaven National Laboratory, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, ALI YAZDANI, Department of Physics, Princeton University — The proximity effect is seen when a superconductor is in contact with a metal. The pairing gap in the superconductor is reduced near the interface while superconducting correlations are induced in the metal. Recent results in high-\( T_c \) superconductor \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \) indicate that the pairing gap closes homogeneously in space, producing a unique state just above \( T_c \) in these compounds where non-superconducting regions are in contact with regions where the pairing gap can still be measured. We will present detailed scanning tunneling measurements that map the local density of states in the same area of the sample from the low temperature fully gapped regime to the high temperature regime where most gaps have closed. We find that the temperature at which the gap closes locally is sensitive to the gaps in the surrounding region.

3 Work supported by NSF, DOE and PCCM-MRSEC.

11:51AM V10.00004 Superconducting Proximity Effect in Thin Semiconducting Films, MICHAEL VISSERS, SOREN FLEXNER, PAUL WELANDER, KEVIN INDERHEES, TIM MCARDLE, JIM ECKSTEIN, University of Illinois at Urbana Champaign — We report results using a novel 3 terminal device structure that provides two independent resistance measurements that we use to examine the influence of the superconducting proximity effect on both the transport properties of the thin film N layer by quantifying its sheet resistance, \( R_s \), as well as independently measuring the junction conductance across the N-S boundary, \( G_c \). When the N layer is a degenerate semiconductor the changes in these quantities are large. \( G_c \) increases much more than the factor of 2 that Andreev Reflection or BTK theory predicts, and both \( G_c \) and \( R_s \) exhibit reentrance as temperature decreases. We interpret these effects as being due to a transition between a phase fluctuating and phase stiff proximity effect in the N layer. This manifests itself by moving the N-S electrical boundary into the semiconductor, increasing \( G_c \), while simultaneously removing volume available to normal transport forcing the measured conductance to increase at a rate that is much faster than the factor of 2 predicted by the model. We find that the pairing gap closes inhomogeneously in space, producing a unique state just above \( T_c \) in these compounds where non-superconducting regions are in contact with regions where the pairing gap can still be measured. We will present detailed scanning tunneling measurements that map the local density of states in the same area of the sample from the low temperature fully gapped regime to the high temperature regime where most gaps have closed. We find that the temperature at which the gap closes locally is sensitive to the gaps in the surrounding region.

12:03PM V10.00005 Charge leakage in superconducting \( \text{La}_2\text{CuO}_4 \) – \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) superlattices, S. SMADICI, P. ABBAMONTE, J. LEE, S. WANG, University of Illinois at Urbana-Champaign, IL 61801, USA, C.D. CAPELLINI, Universite Paris 12 and CNRS UPS-ESPCI, Paris, France, A. GOZAR, G. LOGVENOV, I. BOZOVIC, Brookhaven National Laboratory, NY 11973, USA — Ability of grow crystalline high-temperature superconductor (HTS) superlattices using molecular beam epitaxy has opened new avenues of research. Scanning tunneling microscopy measurements have identified a pronounced influence of the dopant atoms on microscopic properties of bulk HTS, therefore raising the question of whether the holes can be spatially separated in an oxide heterostructure from the disordered doped layers in a way analogous to semiconductor modulation doping. We used resonant soft x-ray scattering (RSXS) to answer this question for \( \text{La}_2\text{CuO}_4 \) – \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) superlattices. For a 15 x 2 x LCO – 4 x LSCO superlattice with \( x=0.36 \), the measured mode amplitude modulation at the \( O \) edge shows a relatively weak localization of the doped holes to the LSCO layers. By using the interference between “structural” and resonant scattering at the \( Cu L_2 \) edge, the c-axis stress of the LSCO sublattice was also observed.

1 Supported by NSF, DOE and PCCM-MRSEC.
12:15PM V10.00006 Long range proximity effect in High Tc Josephson NanoJunctions: a quantitative study

JEROME LESUEUR, NICOLAS BERGEAL1, Physique Quantique, LPEM-CNRS-ESPCI, 10 Rue Vauquelin, 75231 Paris, France, MARCO APRILI, LPS-Universite Paris Sud, Bat 510, 91 405 Orsay Cedex, France, TAKIS KONTOS, LPA ENS, 24 rue Lhomond, 75005 Paris, France, MARTIN SIRENA, Physique Quantique, LPEM-CNRS-ESPCI, 10 Rue Vauquelin, 75231 Paris, France, GIANCARLO FAINI, LPN-CNRS, Route de Nozay, 91460 Marcoussis, France, JEAN-PIERRE CONTOUR, UMR-CNRS/THALES, Route N128, 91120 Palaiseau, France — Proximity effect (PE) between a superconductor S and a normal metal N has been a powerful tool to study conventional superconductors. In High Tc (HTc) compounds, low quality interfaces and poor Fermi wave-vector match with most of metals considerably reduce the PE, and make really difficult its study. We have designed Josephson NanoJunctions in which two S reservoirs are coupled through an N layer at a nanoscale, where N is a lightly disordered HTc, whose Tc has been reduced by ion irradiation. In these SNS junctions, Cooper pairs propagate through the N layer by PE. In this situation with no metallic interfaces within the same material, we have shown that a long range PE takes place, which can be quantitatively described by the diffusive Usadel equations. The Josephson coupling temperature can be computed. The role of the order parameter symmetry will be also discussed.

1Present address: Yale University USA

12:27PM V10.00007 The Superconducting State of Pr$_{2-x}$Ce$_x$Cu$_4$: Tunneling study

YORAM DAGAN, Tel Aviv University, ROY BECK, University of California, Santa-Barbara, RICHARD GREENE, University of Maryland — We report a tunneling study between the electron-doped high Tc, cuprate superconductor Pr$_{2-x}$Ce$_x$Cu$_4$, and Lead as a function of doping, x. Our data fits a nonmonotonic d-wave order parameter for the whole doping range studied. From our data we are able to conclude that the electron-doped cuprate Pr$_{2-x}$Ce$_x$Cu$_4$ is a weak coupling, BCS superconductor in the dirty limit. Phys. Rev. Lett. 99, 147004 (2007)

12:39PM V10.00008 Local tunneling spectroscopy and infrared spectroscopy of the electron-doped cuprate Sm$_{2-x}$Ce$_x$O$_{4+y}$

A. ZIMMERS, [1,2,3], Y. NOAT, T. CREN, W. SACKS, D. RODITCHEV, [1] INSF, Paris, France, B. LIANG, R. L. GREENE, [2] CNAM, Univ of Maryland, USA, R. P. S. M. LOBO, N. BONTEMPS, [1] LPEM, ESPCI, Paris, France — We present infrared and local tunneling spectroscopy of the electron-doped cuprate Sm$_{2-x}$Ce$_x$O$_{4+y}$. In STM, at optimal doping x=0.15, a clear signature of the superconducting gap is observed with an amplitude ranging from place to place and from sample to sample (Δ ~ 3.5-6meV). Another spectroscopic feature is simultaneously observed at high energy above ±50meV. Its energy scale and temperature evolution is found to be compatible with previous photoemission and optical experiments. If interpreted as the signature of antiferromagnetic order in the samples, these results could suggest the coexistence on the local scale of antiferromagnetism and superconductivity on the electron-doped side of cuprate superconductors. Using optical spectroscopy, we analyzed the effects of the normal state gap opening (the higher energy gap seen in STM) and phonon structure as a function of temperature and doping from the underdoped to the metallic composition.

2Support from NSF Grant No. DMR 0352735 and from the German-Israeli Foundation is acknowledged

12:51PM V10.00009 Spin correlations and magnetic excitation spectrum of electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4}$±δ

EUGENIE MOTOYAMA, GUCHUAN YU, YUAN LI, INNA VISHIK, PATRICK MANG, MARTIN GREVEN, Stanford University, OWEN VAJK, University of Missouri - Columbia, KLAUDIA HRADIL, RICHARD MOLE, Forschungsinstitut für Nanoskopie der Universität Hamburg, Hamburg, Germany — We present the results of local tunneling spectroscopy and infrared spectroscopy for electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4}$±δ, one of the most intriguing issues in the field of high-Tc superconductivity is the electron-hole asymmetry: the hole- or electron-doping of the parent Mott insulators leads to superconductors with differing properties. The phase diagram is asymmetric with respect to electron and hole doping, and for the comparatively less-studied electron-doped materials, the role of electronic correlations and nesting are not as clear as for the hole-doping phase. Inelastic neutron scattering measurements have shown the possibility that in the electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4}$±δ, genuine long-range antiferromagnetism and superconductivity do not co-exist (Motoyama et al., Nature 445, 186 (2007)). However, some uncertainty remains, due to the inhomogeneity of Ce concentration x in the large single crystals. Here we report new results using improved homogeneity. In addition to the implications for the phase diagram using energy-integrated measurements, we discussed the impact of improved crystals on the (energy-resolved) magnetic excitation spectrum in the superconducting state.

1This work was supported by NSF Grants Nos. DMR-0352735 and DMR-0303112 at the University of Maryland. A. Z. acknowledges support from I2CAM, NSF Grant No. DMR-0645401.

1:03PM V10.00010 EXAFS study of the role of apical oxygen on superconductivity in Pr$_{0.88}$La$_{0.12}$Ce$_{0.88}$CuO$_{4}$

S. ROSENKRANZ, D. HASKEL, M. BALASUBRAMANIAN, S. HEALD, Argonne National Laboratory, S. LI, P. DAI, University of Tennessee and ORNL, Y. ANDO, CRIEPI — One of the longstanding puzzles surrounding high-Tc cuprates concerns the apparent asymmetry between electron and hole doping. Whereas hole doping quickly superconductivity, electron doping alone in materials such as Pr$_2$CuO$_y$ is insufficient and superconductivity is only achieved after a high temperature, low-oxygen annealing. While it was believed that this annealing process removes small amounts of oxygen in apical positions assumed to induce localization of the doped electrons, this scenario is incompatible with Raman, infrared- transmission, and ultrasound studies. In contrast, based on synchrotron X-ray and neutron diffraction studies combined with chemical and thermo-gravimetric analysis measurements, we recently showed that the annealing process alleviates minor Cu- deficiencies present in the as-grown sample. Here we present EXAFS studies on powder and single-crystal samples of as-grown and annealed Pr$_{0.88}$La$_{0.12}$Ce$_{0.88}$CuO$_{4}$. Our results are consistent with no change in the occupation of apical oxygen between the superconducting and as-grown samples, providing further evidence that the main effect of the annealing process is to repair defects in the superconducting planes due to Cu- deficiencies present in as grown samples. Work supported by US DOE BES-DM5 DE-AC02-06CH11357

1:15PM V10.00011 High pressure study on Pr$_{1.85}$Ce$_{0.15}$CuO$_{4}$−δ single crystals

COSTEL R. ROTUNDU, Department of Physics, University of Maryland, College Park, MD 20742, USA, VIKTOR V. STRUZHKIN, ALEXANDER GONCHAROV, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA, RICHARD L. GREENE, Department of Physics, University of Maryland, College Park, MD 20742, USA — Transport measurements to 2.5 GPa on electron-doped cuprates revealed modest changes in physical properties, if any [1]. Room temperature synchrotron diffraction on powder samples show that the non-superconducting parent Pr$_2$CuO$_4$ exhibits a gradual structural transition from T’ to T phase when subject to pressures greater than 15 GPa [2]. Pr$_{2-x}$Ce$_x$CuO$_4$ (PCCO) is superconducting for a Ce doping range 0.12 – 0.2 (T’ structure). Both pressure and Tc have been reduced by ion irradiation. In these SNS junctions, Cooper pairs propagate through the N layer by PE. In this situation with no metallic interfaces within the same material, we have shown that a long range PE takes place, which can be quantitatively described by the diffusive Usadel equations. The Josephson coupling temperature can be computed. The role of the order parameter symmetry will be also discussed.

1:27PM V10.00012 Recent ARPES results on electron-doped high-Tc superconductors and comparison to their hole-doped counterparts. PIERRE RICHARD, ZHIHUI PAN, MADHAB NEUPANE, YIMING XU, Boston College; PATRICK FOURNIER, Université de Sherbrooke, SHILIANG LI, PENGCHENG DAI, University of Tennessee, Knoxville, ZIQIANG WANG, HONG DING, Boston College — Since the CuO2 planes of cuprates, where high-temperature superconductivity occurs, can be doped either by holes or electrons, it appears important to establish similarities between these two types of doping in order to have an overview of high-temperature superconductors, especially for the electronic structure. Hence, although much less studied by ARPES than their hole-doped counterpart, the electronic structure of the electron-doped cuprates is believed to provide essential hints towards the understanding of high-Tc superconductivity. We present our recent ARPES results on electron-doped cuprates, focusing on various ranges of energy. We compare the results to those obtained on commonly studied hole-doped cuprates.

1:39PM V10.00013 Point contact tunnelling as a probe for the superconducting properties of Niobium RF cavities. T. PROSLIER, J. MOORE, Argonne Nat. Lab., J. ZASADZINSKI, Illinois Inst. Tech., M. PELLIN, J. NOREM, Argonne Nat. Lab., MSD TEAM, HEP TEAM, IIT TEAM — Niobium, with its very high Hc2, has been used in superconducting RF cavities for accelerator systems for 40 years with continuous improvement. The quality of cavities (Q) is governed by the surface impedance RBCS, which depends on the quasiparticle gap, \( \Delta \), and the superfluid density, \( n_s \). Both of these parameters are seriously affected by surface imperfections (metallic phases, dissolved oxygen, magnetic impurities). Surface treatments of Nb cavities improved the Q factor, but are not understood from a fundamental point of view. Point contact tunneling spectroscopy is an ideal, surface sensitive probe as the quasiparticle current measures \( \Delta n \). We present some measurements on SRF cavity-grade Nb using point contact tunneling demonstrating that the nature of the Nb oxide has a significant effect on \( \Delta \). Atomic Layer Deposition was used to grow an alumina oxygen diffusion barrier on Nb providing control of the Nb oxidation layer composition with subsequent annealing. Point contact tunneling on these samples help to unravel the complicated effect of Nb surface oxidation on \( \Delta \).

1:51PM V10.00014 Scanning Tunneling Microscopy of Defect-Induced Superstructure in 2H-NbSe2. HUI WANG, JONGCHEE LEE, MICHAEL DREYER, U of Maryland, College Park, BARRY BARKER, Laboratory of Physical Sciences — Scanning tunneling microscopy and spectroscopy measurements were performed on pure 2H-NbSe2 with defects introduced by tip-sample interaction at 4K. Domains of a new superstructure with a lattice constant equals \( \sqrt{3} a_0 \) instead of \( 3 a_0 \) were observed around the defects. Closer to the defects we also observed the disordered phase of this structure. Both of them are stable under the STM measurements at 4K. Atomically resolved microscopy and spectroscopy studies suggest a 2H to 1T phase transition induced by surface atom sliding.

2:03PM V10.00015 STM Investigation of Bosonic Modes and a Superconducting Gap in the Electron Doped Cuprate Pr1−xLaCe2CuO4. FRANCIS NIESTEMSKI, SHANKAR KUNWAR, SEN ZHOU, Boston College, SHILIANG LI, University of Tennessee, Knoxville, HONG DING, ZIQIANG WANG, Boston College, PENGCHENG DAI, U Tennessee, Knoxville & ORNL, VIDYA MADHAVAN, Boston College — While continual effort in scanning tunneling microscopy (STM) remains focused on the hole-doped cuprates less attention has been given to the equally important electron-doped side of the phase diagram. We use a variable temperature UHV STM to investigate the electron-doped cuprate superconductor Pr1−xLaCe2CuO4. We explore temperatures 2 K and higher and find a superconducting gap that disappears above Tc. We also find satellite features anti-correlated to the gap which we associate with bosonic modes. We relate our findings to neutron scattering results and discuss how this electron doped superconductor differs from more familiar hole-doped cuprates.


11:15AM V11.00001 Evidence of Electron Coupling to High Energy Excitations in a High Temperature Superconductor. XINGJIANG ZHOU, WENTAO ZHANG, GUODONG LIU, LIN ZHAO, HAIYUN LIU, JIANQIAO MENG, XIAOLI DONG, WEI LU, ZHONGXIAN ZHAO, GUILING WANG, HONGBO ZHANG, YONG ZHOU, ZUYAN XU, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, YONG DING, ZIQIANG WANG, Boston College, PENGCHENG DAI, U. of Maryland, College Park, BARRY BARKER, Laboratory of Physical Sciences — Scanning tunneling microscopy and spectroscopy measurements were performed on pure 2H-NbSe2 with defects introduced by tip-sample interaction at 4K. Domains of a new superstructure with a lattice constant equals \( \sqrt{3} a_0 \) instead of \( 3 a_0 \) were observed around the defects. Closer to the defects we also observed the disordered phase of this structure. Both of them are stable under the STM measurements at 4K. Atomically resolved microscopy and spectroscopy studies suggest a 2H to 1T phase transition induced by surface atom sliding.

11:27AM V11.00002 High energy kink in the single particle spectra of the two-dimensional Hubbard model. ALEXANDRU MACRIDDIN, MARK JARRELL, University of Cincinnati, THOMAS MAIER, Oak Ridge National Laboratory, DOUGLAS SCALAPINO, University of California, Santa Barbara — Employing dynamical cluster quantum Monte Carlo calculations we show that the single particle spectral weight \( \omega(k,\omega) \) of the one-band two-dimensional Hubbard model displays a high energy kink in the quasiparticle dispersion followed by a steep dispersion of a broad peak similar to recent ARPES results reported for the cuprates. Based on the agreement between the Monte Carlo results and a simple coupling which calculates the quasiparticle to spin fluctuations, we conclude that the kink and the broad spectral feature in the Hubbard model spectra is due to scattering with damped high energy spin fluctuations.

11:39AM V11.00003 Theory of quasiparticle excitations in cuprates: universal Fermi velocity and high energy anomalies. QIANG-HUA WANG, Nanjing University — Recent measurements of quasiparticles in hole-doped cuprates reveal highly unusual features: 1) the doping-independent Fermi velocity, 2) two energy scales in the quasiparticle spectral function, and 3) a suppression of the low energy spectral weight near the zone center. The underlying mechanism is under hot debate. We addressed these important issues by a new mean field theory and a novel variational Monte Carlo (VMC) study of the \( t-J \) model. We obtained results in both approaches in agreement with the experiments but without invoking extrinsic effects. They reflect the role of strong correlations in the form of local Mottness and antiferromagnetic fluctuations, yielding a strong connection between the low and high energy quasiparticle excitations. Besides, we resolved a long standing issue of the sum rule for quasiparticle spectral weights in traditional VMC studies. The electron doped case was also discussed and we concluded that no high energy anomaly exists in the occupied side, in contrast to the hole doped case.
11:51AM V11.00004 Dispersion and spectral weight analysis of “waterfall” structure in Pb doped Bi2212. QIANG WANG, ZHE SUN, ELI ROTENBERG, HELMUT BERGER, DANIEL DESSAU — Angle resolved photoemission spectroscopy (ARPES) is used to investigate the property of the “waterfall” structure in (Bi, Pb)2Sr2CaCu2O8+δ. The dispersion analysis of the spectrum shows that there is not a “universal high energy scale” in this material. And the spectral weight analysis suggests that the matrix element and the inelastic scattering may have an important role in the formation of the waterfall structure.

12:03PM V11.00005 Magnon Corrections to Cuprate Self Energy1, ROBERT MARKIEWICZ, TANMOY DAS, ARUN BANSIL, Northeastern University — Recently, high energy kinks (‘waterfalls’) have been reported above 200 meV in the ARPES spectra of several cuprates. These kinks are a signal of bosonic coupling and may be responsible for the band renormalizations found at lower energies. We have shown that coupling to collective modes in the spin channel can yield waterfall-like effects in the electronic dispersion in the electron as well as hole doped cuprates. [1] Here we further explore the effects of the magnons in the pseudogap regime, including a discussion of how magnons influence optical properties. [1] R.S. Markiewicz, S. Saharakori, and A. Bansil, cond-mat/0701524, to be published, PRB.

1 Work supported in part by the DOE.

12:15PM V11.00006 Aspects of the electron-phonon interaction in the Cuprates, STEVE JOHNSTON, University of Waterloo, WEI-SHENG LEE, THOMAS DEVEREAUX1, Z.X. SHEN, Stanford University — The ubiquity of the “kink”-structures observed in the band-dispersion of the High-Tc cuprates has made this feature the subject of debate for many years now. At present, the community agrees that the feature is due to electron-boson coupling to a collective mode, however, a consensus has yet to be reached on its identity. In this talk we will review the arguments typically made against the phonon interpretation, which are grounded in knowledge gained from metallic systems. We will then show the complications one encounters in extrapolating from these systems to strongly correlated systems such as the cuprates. We will also discuss some of the common methods for extracting information from photoemission spectra that are cited in the modern literature in order to highlight the strengths and weaknesses of each and their reliability for extracting realistic estimates for parameters such as the electron-boson coupling strength λ.

1 Also affiliated with the Stanford Linear Accelerator Center

12:27PM V11.00007 Phonon anomaly in Bi2Sr2CaCu2O8+δ,* JIANDONG GUO, HUAJUN QIN, KEHUI WU, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, R. G. MOORE, E. W. PLUMMER, University of Tennessee, Knoxville, TN 37996, J. WEN, G. D. GU, Brookhaven National Lab, Upton, NY 11973, JIANDI ZHANG, Florida International University, Miami, FL 33199 — Electron-phonon coupling (EPC) plays in many exotic phenomena displayed by strongly-correlated electron materials, such as the pairing mechanism in high-Tc superconductors and metal-insulator transition in ruthenates. Many studies show a strong renormalization of quasi-particle band structure near Fermi energy associated with the coupling to boson modes ~40-50 meV. However, there is no clear picture of the origin of these modes. With angle-resolved electron energy loss spectroscopy, we have studied the lattice dynamics of Bi2Sr2CaCu2O8+δ surface. The data indicate a phonon anomaly of modes ~50 meV, identified as the in-plane Cu-O stretching modes, where the energy shifts (softens) while the spectral linewidth and weight vary along (0,0)-(π,0) direction. The other feature ~80 meV, attributed to apical oxygen vibrations, exhibits distinct dispersion toward (π,π). Such behaviors are observed both above and below the superconducting Tc. These detailed measurements provide new insights into the nature of EPC in such materials. * Supported by China NSF-10704084, NSF DMR-0346826, NSF and DOE (NSF-DMR-0451163 and DMS&E).

12:39PM V11.00008 Isotope effect on the nodal kink energy in Bi2212, J.F. DOUGLAS, University of Colorado, Boulder, H. IWASAWA, Tokyo University of Science, National Institute of Advanced Industrial Science and Technology, K. SATO, H. EISAKI, Y. YOSHIDA, H. BANDO, — Using low energy angle resolved photoemission spectroscopy (le-ARPES), we have observed an energy shift of the nodal kink upon substitution of 18O for 16O in optimally doped (Tc ~92K) Bi2Sr2CaCu2O8+δ. Studying several samples of each isotope, we find that the kink energy decreases by 3.22 ± 0.72 meV upon 18O substitution, in good agreement with the energy shift one would expect from a phononic mode. This strongly supports the view that the nodal dispersion kink arises from electronic coupling to a phononic mode.


1:03PM V11.00010 Fermi Surface Topology Effects on the Electron-Phonon Coupling in Electron-doped Cuprates, S.R. PARK, D.J. SONG, C.S. LEEM, CHUL KIM, C. KIM1, Institute of Physics and Applied Physics, Yonsei University, Seoul, Korea, B.J. KIM, School of Physics and Center for Strongly Correlated Materials Research, Seoul National University, Seoul, Korea, H. EISAKI2 — We have performed high resolution angle resolved photoemission (ARPES) studies on electron doped cuprate superconductors Sm2−xCexCuO4 (x=0.10, 0.15, 0.18). Imaginary parts of the electron removal self energy for a newly developed method show kink-like features due to electron-bosonic mode coupling. The kink-like feature is seen along both nodal and anti-nodal directions but at different energies of 50 and 70 meV. Such energy scales can be reconciled by taking the Fermi surface topology and phonon dispersions into account, revealing the kink structures are due to the electron-phonon coupling. Estimated electron-phonon coupling constant λ from the self energy is about 0.6 independent of doping and is isotropic. In addition to the low energy feature, we observe a hump structure at 350 meV which is anisotropic and exists only in the anti-nodal spectrum.

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1:15PM V11.00011 Theoretical fits of laser-ARPES energy distribution curves of the high Tc superconductor Bi2212. N.C. PLUMB, University of Colorado, P.A. CASEY, Princeton University, J.D. KORALEK, LBNL and UC Berkeley, J.F. DOUGLAS, Z. SUN, University of Colorado, Y. AIURA, K. OKA, H. EISAKI, AIST Tsukuba, P.W. ANDERSON, Princeton University, D.S. DESSAU, University of Colorado — Laser-ARPES has produced spectral lineshapes in photoemission that are much sharper than any previous data, which is due to increased energy and momentum resolution, increased bulk sensitivity, and decreased final state broadening. The lifetimes of these states, extracted from simple Lorentzian fits to the data, are consistent with bulk-sensitive optical data, implying that we are for the first time measuring the intrinsic spectral function. It therefore is appropriate to study the spectral lineshape in detail. We have looked at standard Lorentzian energy distribution curves, as well as extensions based upon Fermi Liquid theory, Marginal Fermi Liquid theory, and of great interest, a non-Fermi Liquid theory based upon Anderson’s treatment of the Gutzwiller projection. The lineshapes based upon the Gutzwiller projection utilize only one free parameter and include no background term, yet they fit the data well over a broad range of temperatures and energies.

1:27PM V11.00012 Properties of high-Tc superconductors from spin-phonon coupling and band models. THOMAS JARLSTORP, DPMC, University of Geneva, CH1211 Geneva 4, Switzerland — An understanding of the rich doping- and \((q, \omega)\)-dependences of spin excitations in high Tc materials is essential since the mechanism of high-Tc superconductivity might be linked to spin fluctuations. Ab-initio band calculations show important spin-phonon coupling (SPC), i.e. antiferromagnetic fluctuations are enhanced when they co-exist with \(q\)-phonons involving O, Cu or La distortions. Parameters for these “1-dimensional” (1D) electron-phonon and spin-wave couplings are obtained from band calculations for long supercells containing phonon distortions and/or staggered fields. The characteristic 2-D q-dependence of the excitations are calculated for a free-electron like band with the use of the ab-initio parameters. The q-dependence depend on the strength of the SPC. The SPC is strongest for in-plane O-modes, weaker for modes involving the heavy atoms, and smallest for apical O, which together with SPC for the phonons at the characteristic frequency lead to a \(q\)-dependent excitation spectrum. These and other properties coming from SPC in the band/free-electron model compare favorably with observations.

1:39PM V11.00013 Universal dispersion anomalies revealed by DQMC simulations of the Hubbard model. B. MORITZ, SLAC, S. JOHNSTON, U. Waterloo, W. MEEVASANA, Stanford U., C. KIM, Yonsei U., T. P. DEVEREAUX, Stanford U. and SLAC, R. T. SCALETTER, UC Davis, Z.-X. SHEN, Stanford U. and SLAC — The recent observation of a “high energy anomaly” (HEA) in hole-doped high-Tc compounds, as well as the half-filled parent insulators, using angle-resolved photoemission spectroscopy (ARPES) has sparked a great deal of interest and intense theoretical and experimental investigations. Using determinant quantum Monte Carlo (DQMC) and maximum entropy analytic continuation (MEM), we investigate the existence of HEA in the single-band Hubbard model. The spectral functions obtained from the simulations reveal a universal HEA across the doping spectrum, similar to that seen in experiment. This signals a cross-over from a quasiparticle-like band at low energy to the incomherent lower Hubbard band at higher energy. A comparison of the self-energy obtained from simulation to that extracted from experiment serves as a further illustration of the similarities. In addition, we perform simulations of the single-band Hubbard model on the electron-doped side of the phase diagram and compare and contrast our results to existing experimental evidence and comment on the possibility that future experiments would find a universal HEA in electron-doped compounds.

1:51PM V11.00014 Local effects of apical oxygen on superconductivity in high-\(T_c\) cuprates. MICHYASU MORI, Tohoku Univ., TAKAMI TOHYAMA, Kyoto Univ., SADAMICHI MAEKAWA, Tohoku Univ. — The superconducting critical temperature \((T_c)\) of high-\(T_c\) cuprates widely distributes among various series of crystal structures, even if the doping rate is optimized in the \(\text{CuO}_2\) planes. In addition, the \(T_c\) is enhanced by applying pressure[1]. These material- and pressure dependences have meaningful correlation with an energy difference of oxygen sites in an apical site and in the \(\text{CuO}_2\) plane \((V_A)\)[2]. On the other hand, Slezak et al. has found that locally modulated gap energy has anti-correlation with a distance between a \(\text{Cu}\) and an apical O-sites, i.e., the larger distance is related to the smaller gap energy[3]. We study such a local effect of apical oxygen on superconductivity by calculating the Madelung potential. In particular, we focus on a local variation of \(V_A\), whose value approximately corresponds to stability of the Zhang- Rice singlet state[2]. It is found that, on neighboring sites of apical sites close to Cu sites, \(V_A\) are locally enhanced compared to other sites. To estimate the gap energy, we propose a toy model like a BCS mean field Hamiltonian with an additional degree of freedom, which describes a role of apical oxygen. These material and pressure variations have meaningful correlation with an energy difference of oxygen sites and gap energy, which approximately corresponds to stability of the Zhang- Rice singlet state[2]. In the future, this effect will be studied on the same system in experiment.

2:03PM V11.00015 Variable Temperature Scanning Tunneling Spectroscopy of Inhomogeneous High Temperature Superconductors. E.W. HUDSON, M. C. BOYER, W.D. WISE, KAMALES CHATTERJEE, YAYU WANG, MIT, TAKESHI KONDO, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, TSUNEHIRO TAKEUCHI, HIROSHI IKUTA, Nagoya University — Scanning Tunneling Microscopy (STM) of the high temperature superconductor \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}\) (Bi-2212) long ago revealed large gap variations on nanometer length scales. In this talk I will discuss new results from our temperature dependent STM studies of Bi-2201. In particular, I will focus on the effects of these variations on other observables, such as the states generated around single atom impurities, as well as on other measurement techniques, such as angle resolved photoemission (ARPES).

Thursday, March 13, 2008 11:15AM - 2:03PM – Session V12 DCMP: Metal Insulator Transition I: Vanadium Oxides and Others Morial Convention Center 203

11:15AM V12.00001 Electrical measurements at the metal-insulator phase boundary in \(\text{VO}_2\) nanobeams1. DAVID COBDEN, JIANG WEI ZENGHUI WANG, WEI CHEN, University of Washington — We study the electrical properties of vanadium dioxide nanobeams undergoing the metal-insulator transition (MIT), which occurs at a temperature of \(67^\circ\text{C}\) at ambient pressure. The nature of the MIT in bulk \(\text{VO}_2\), although known to involve electron-electron correlations, has remained elusive since its discovery fifty years ago. In nanobeams clamped at both ends there is a coexistence regime which allows electrical measurements along the phase boundary. Remarkably, the resistivity of the insulating phase turns out to be constant along the phase boundary implying that the transition is driven by electron density, consistent with a Mott-type mechanism. The measurements show that the resistance of a domain wall is negligible, and the resistance of a nanowire gives a direct measure of the length of insulating phase present in the wire, allowing one to study the motion of the domain wall electrically with high precision.

1 This work was supported by the Army Research Office.
11:27 AM V12.00002 Metal-insulator coexistence in VO$_2$ nanobeams$^1$. JIANG WEI, ZENGHUI WANG, WEI CHEN, DAVID COBDEN, University of Washington — We study the first-order metal-insulator transition (MIT) in vanadium dioxide nanobeams. The MIT occurs sharply at a temperature of $T_c = 67^\circ C$ at ambient pressure. However, in nanobeams clamped at both ends, and hence subjected to a constant length condition, there is a wide coexistence regime between the two phases, which can be visualized in an optical microscope. Above $T_c$, the beam is under axial tension and on warming up follows the phase boundary in the tension/temperature plane. Below $T_c$, the beam buckles under compressive strain. The metallic phase can be supercooled by up to 50°C. Usually there is a single metal-insulator domain wall in each beam, but a mobile bubble-like insulating domain can be induced by applying a nonuniform temperature profile.

$^1$This work was supported by the Army Research Office.

11:39 AM V12.00003 Correlation between metal-insulator transition characteristics and electronic structure changes in vanadium oxide thin films, D. RUZMETOV, V. NARAYANAMURTI, S. RAMANATHAN, SEAS, Harvard University, Cambridge, MA, S.D. SENANAYAKE, CSD, Oak Ridge National Lab, Oak Ridge, TN — We correlate electron transport data with energy band structure measurements in vanadium oxide thin films with varying V-O stoichiometry across the VO$_2$ metal-insulator transition (MIT). A set of vanadium oxide thin films were prepared by reactive DC sputtering from a V target at various oxygen partial pressures resulting in films with different MIT strength as determined from the electrical resistance measurements. The results of the near edge X-ray absorption fine structure spectroscopy (NEXAFS) of the O K-edge in identical VO films are presented. Redistribution of the spectral weight from $\sigma^*$ to $\pi^*$ bands is found in the vanadium oxide films exhibiting stronger VO$_2$ MIT. This is taken as evidence of the strengthening of the metal-metal ion interaction with respect to the metal-ligand and indirect V-O-V interaction in vanadium oxide films featuring sharp MIT. We observe also a clear correlation between MIT and the width and the area of the lower $\pi^*$ band which is likely to be due to the emergence of the $d_{1\bar{g}}$ band overlapping with $\pi^*$. The strengthening of this $d_{1\bar{g}}$ band near the Fermi level only in the vanadium oxide compounds displaying the MIT points out the importance of the role of the $d_{1\bar{g}}$ band and electron correlations in the phase transition.

11:51 AM V12.00004 Mott transition in vanadium dioxide (VO$_2$) observed by infrared spectroscopy and nano-imaging$^1$, M.M. QAZILBASH, G.O. ANDREEV, D.N. BASOV, P.C. HO, M.B. MAPLE, Physics Department, University of California - San Diego, M. BREHM, F. KEILMANN, Abt. Molekulare Strukturbiologie, Max-Planck-Institut fur Biochemie and Center for NanoScience, A.V. BALATSKY, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, BONG-JUN KIM, SUN JIN YUN, HYUN-TAK KIM, IT Convergence And Components Lab, ETRI, Daejeon, Korea — The driving mechanism for the temperature-induced insulator-to-metal transition (MIT) in vanadium dioxide (VO$_2$) has been debated for the past five decades. Central to this debate is the relative importance of electron-electron correlations and charge-ordering to the MIT. We report near-field infrared images of VO$_2$ films that directly show the percolative MIT. In combination with far-field infrared spectroscopy, the new data reveal the Mott transition with divergent optical mass in the metallic puddles that emerge at the onset of the MIT.

$^1$This work was supported by the US Department of Energy, the DFG Cluster of Excellence Munich-Centre for Advanced Photonics, and the High Risk High Return project in ETRI, Korea.

12:03 PM V12.00005 Avalanches in the Metal-Insulator transition in Vanadium Oxide nanoscaled junctions, AMOS SHARONI, GABRIEL RAMIREZ$^1$, IVAN K. SCHULLER, University of California, San Diego — We present transport measurements on sub-micron devices of VO$_2$. Instead of the usual smooth metal insulator transition, we observe for the first time multiple resistive steps. The temperature driven transition between the two phases occurs through a series of avalanches of different amplitude, ranging over 2 decades of resistance. The data is analyzed assuming a generic normalized probability distribution. Results are similar to those obtained in martensitic transitions or Barkhausen noise in ferromagnets, implying universality of first order phase transition. We will discuss the distribution of resistance avalanches as a function of temperature caused by the percolative nature of resistive transition. In particular we will focus on the effect of the VO$_2$ junction dimensions and the transport measurement conditions (such as applied current and temperature ramp rate) on the results. Work supported by the US –Department of Energy.

$^1$On leave from Universidad del Valle, Cali, Colombia.

12:15 PM V12.00006 Micro X-Ray Diffraction Study of VO$_2$ Films – Separation between Metal-Insulator Transition and Structural Phase Transition, KIM HYUN-TAK, KIM BOUNG-JUN, ETRI in Korea, LEE YONG WOOK, ETRI in Korea, YUN SUN JIN, LIM JUNG-WOOK, ETRI in Korea, SHIN TAE-JU, POSTEC, YOUN HWA-SICK, POSTECH — It has been well-known that VO$_2$ undergoes both a structural phase transition (SPT) from monoclinic (insulator phase) to tetragonal (metal phase) and a discontinuous first-order metal-insulator transition (MIT) (Jump) near 68°C. When the MIT and the SPT occurs simultaneously, the MIT can be regarded as the Peierls transition. When both take place separately, the MIT can be interpreted as the Peierls transition. Peierls transition and Mott transition in VO$_2$ remain controversial. We have investigated a relation of the MIT and the SPT which are simultaneously measured by I-V measurement and synchrotron micro X-ray of the 1B2 line in Pohang accelerator Lab., respectively. A used sample is a VO$_2$-based two terminal device. The result shows that the MIT and the SPT does not occur simultaneously. (References on the MIT: New J. Phys. 6 (1994) 52 (http://www.njp.org), Appl. Phys. Lett. 86 (2005) 242101, Physica B 369 (2005) 76, Phy. Rev. Lett. 97 (2006) 266401, Appl. Phys. Lett. 90 (2007) 023515).

12:27 PM V12.00007 Lateral V/VO$_2$/V Tunnel Junctions Formed by Anodic Oxidation, DAVID KIRKWOOD, KEVIN WEST, JIWEI LU, STUART WOLF, University of Virginia — Anodization has been found to be a simple and cost effective technique to produce oxide films of many transition metals. In this work, we have used anodic oxidation as a means of fabricating lateral V/VO$_2$/V junctions. Vanadium wires grown by ion beam deposition were patterned by lithography and an active working window was defined on the wire. VO$_2$ was then grown under galvanostatic control in a two electrode electrochemical micro-cell. A droplet of oxygen rich saturated Boric acid was used as the electrolyte to electrically connect the Vanadium working electrode to a Platinum wire counter electrode. A constant current of approximately 100 $\mu$A/cm$^2$ was maintained through the cell for various amounts of time. Electrical measurements of the resulting V/VO$_2$/V junctions indicate a metal to insulator transition (MIT) near 340 K that is similar to the structural phase transition and accompanied MIT of VO$_2$ which occurs at this temperature. A 4-fold change in resistance is observed in the junctions. Below this transition temperature a typical junction behavior is observed with a dramatic change in resistance state from high to low with increasing applied current. This non-linear IV characteristic on the junction with a size of 5 $\mu$m by 15 $\mu$m suggests that the anodized VO$_2$ film behaves like a tunneling barrier.
12:39PM V12.00008 The metal to insulator transition in correlated materials – exchange of low and high energy spectral weight, STEFAN G. SINGER, B. SCHULZ, I. MAHNS, M. BASTJAN, G. NEUBER, A. GOOS, P. SAICHU, S. BINDER, A. RUSYDI, K. HORN, S. ELLER, M. RUBHAUSEN, University of Hamburg, G. STRYGANYUK, HASYLAB/DESY, L. COOPER, UIUC, G.A. SAWTZKY, UBC, O. SUSHKOV, University of New South Wales, H. EISAKI, Y. FUJIMAKI, S. UCHIDA, University of Tokyo, K. DÖRR, IFW — The electronic response of correlated system of manganites and cuprates was investigated by a combination of dc conductivity, ellipsometry, and VUV-reflectance covering an energy range from 0 to 22 eV. By performing a stabilized Kramer-Kronig transformation, we obtain the optical conductivity as a function of temperature around the metal to insulator transition. Our main findings are that changes in the kinetic energy exceed energies of more than 22 eV. Within this range we can establish, that high energy spectral weight gets transferred to low energies into the Drude region. We argue that our findings are general phenomena of correlated materials and outline different scenarios to explain our observations.

12:51PM V12.00009 Metal-insulating transition and Zhang-Rice singlets in one-dimensional cuprates: the case of Ca_{2+x}Y_{2-x}Cu_{x}O_{10}²⁺, ALESSIO FILIPPETTI, VINCENZO FIORENTINI, University of Cagliari, Italy — Chain-like Ca_{2+x}Y_{2-x}Cu_{x}O_{10}²⁺ is the ideal prototype of dopable one-dimensional cuprate with zig-zag Cu-O interactions. The observed abundance of Zhang-Rice singlets in the electronic ground state of the system induces peculiar phase transitions in magnetic and conducting properties upon doping. With the use of unconventional first-principles calculations suitors for to the study of strong-correlated materials, we describe the change of electronic and magnetic properties as doping is varied from x=0 to full-doped concentration (i.e. one hole each Cu_{2}O unit). Zhang-Rice singlets are key ingredients to understand the behavior of doped CuO2 units and the rise of high-Tc superconductivity in cuprates. We can visualize ZR singlets in space and energy at varying doping concentration, and their influence on magnetic and dielectric properties. ZR singlets are associated to holes localization on the oxygens, appear for holes concentration above 0.25 per CuO_{2} and persist up to maximum doping (i.e. one hole per CuO_{2}) that is well above the threshold of the metallic regime. Our findings are indicative of the general behavior of low-dimensional doped cuprates and give evidence that first-principles band-energy approaches can be valuably employed to the study of doped cuprates.

1:03PM V12.00010 EXAFS and XANES in Fe_{3−x}M_{x}O_{4}, M = Zn, Ti, Al with 0 ≤ x < 0.065.
J. SABOL, Chemical Consultants, Racine WI, USA, D. OWOC, Z. KAKOL², C. KAPUSTA, A. KOZLOWSKI, AGH-UST, Krakow, Poland, J. HONIG, Purdue Univ., West Lafayette IN, USA — We present an extended EXAFS and XANES study at the Fe K edge of the local structural changes in Fe_{3−x}M_{x}O_{4}, M = Zn, Ti, Al, with x within the first and second order Verwey transition regimes. The aim of this work was to investigate how the local Fe symmetry is altered at the transition, in view of the drastic change of the overall crystal structure. A comparison of the interatomic distances and Debye-Waller factors shows that the local Fe O-structure around either the octahedral or tetrahedral Fe atoms in magnetite remains nearly unaltered crossing the Verwey transition. This is also independent of the level of doping and dopant ion, i.e., independent of lattice parameters, as Zn and Ti increase the unit cell volume and Al decreases the unit cell volume. Therefore, the local distortion of Fe sites is not a parameter sensitive enough to elucidate the mechanism of the Verwey transition and the change of its character. An examination of different factors, other than local order, is needed to explain the apparent charge ordering below the Verwey transition temperature T_{V}.

1:15PM V12.00011 Nonequilibrium Relaxations and Aging Effects near a Metal-Insulator Transition in Two Dimensions.
DRAGANA POPOVIĆ, JAN JAROSZYŃSKI, NHMFL/FSU — The relaxations of conductivity σ(t) have been studied in the glassy regime of a strongly disordered two-dimensional (2D) electron system in Si after a temporary change of carrier density n_{s} during the waiting time t_{w}. Two types of response have been observed: (a) monotonic, where relaxations exhibit aging, i.e. dependence on history, determined by t_{w} and temperature; (b) nonmonotonic, where a memory of the sample history is lost. The conditions that separate the two regimes have been determined. A detailed study of the aging regime [2] reveals an abrupt change in the nature of the glassy phase at the metal-insulator transition (MIT) before it vanishes entirely at a higher density n_{g}. Our results provide further support to theories describing the 2D MIT as the melting of a Coulomb glass, and put constraints on the models of glassy freezing.

1:27PM V12.00012 Photo-induced Metallic States in a Mott Insulator, TAKASHI OKA, University of Tokyo, Department of Tokyo — In the presence of strong AC electric fields, carriers are continuously produced in an insulator and the system may turn metallic. Such photo-induced insulator-to-metal transition was observed in one-dimensional Mott insulators (Iwai et al. P.R.L. (2003)). We have studied the one-dimensional Hubbard model with strong AC electric fields using the time-dependent density matrix renormalization group method. We have changed the strength of the field as well as the frequency. We have observed that metallic states are produced not only when the photon energy, i.e., the frequency of the AC field, is larger than the gap, but also when it is smaller. However, the field must be stronger than a threshold in the latter case. We have also studied the detailed properties of the photo-induced states by calculating the optical and magnetic correlation function.

1:39PM V12.00013 I³⁺-Ir⁴⁺ Charge Disproportionation of Spinel CuIr₂S₄ investigated by Synchrotron Radiaton Photoemission.
HAN-JIN NOH, E.-J. CHO, Dep. of Phys., Chonnam National University, H.-D. KIM, J.-Y. KIM, Pohang Accelerator Laboratory, POSTECH, C.-H. MIN, School of Phys. and Astron., Seoul National University, B.-G. PARK, Dep. of Phys. POSTECH, S.-W. CHEONG, Rutgers Center for Emergent Materials, Rutgers University — We have studied the electronic structure of the spinel CuIr_{2}S_{4} using synchrotron-radiation photoemission spectroscopy. The phase transition from a high temperature paramagnetic metal to a low temperature diamagnetic insulator at ~230 K is clearly observed through the significant line shape change of the Ir 4f photoemission spectra and the ~0.09 eV gap opening of the valence band spectra. The photon energy dependence of the Ir 4f photoemission spectra enable us to characterize the satellite peaks in the metallic phase of CuIr₂S₄, providing compelling experimental evidence for the Ir³⁺-Ir⁴⁺ charge disproportionation in CuIr₂S₄.
11:15AM V13.00001 Dielectric Properties of Ice and Liquid Water from First Principle Calculations 1, DEYOU LIU, FRANCOIS GYGI, GIULIA GALLI, UC Davis — We present a first-principle study of the dielectric properties of ice and liquid water. The eigenmodes of the dielectric matrix, \( \epsilon^{-1} \), are analyzed in terms of maximally localized dielectric functions similar, in their definition, to maximally localized Wannier orbitals obtained from Bloch eigenstates of the electronic Hamiltonian. We show that the lowest eigenmodes of \( \epsilon^{-1} \) are localized in real space and can be separated into groups related to the screening of lone-pairs, intra-, and inter-molecular bonds, respectively. The local properties of the dielectric matrix can be conveniently exploited to build approximate dielectric matrices for efficient, yet accurate calculations of quasiparticle energies.

1This work was supported by DOE SciDAC grant DE-FC02-06ER25794.

11:27AM V13.00002 Strong hybridization of Frenkel excitons in Mott insulators: a novel Wannier function perspective*, CHI-CHENG LEE, Brookhaven National Laboratory, H. C. HSUEH, Tamkang University, WEI KU, Brookhaven National Laboratory — Linear response scheme of the time-dependent density-functional theory (TDDFT) has been quite successful in the study of the excitations of weakly correlated systems. However, its applicability to strongly correlated systems remains unclear, especially due to the poor quality of the exchange-correlation kernel essential for those systems. On the other hand, the local-density approximation + Hubbard U (LDA+U) approximation has been shown to describe quite successfully the ground-state properties and electronic band structures of Mott insulators. Therefore, it is timely to investigate the linear response of the LDA+U functional in the framework of TDDFT in describing excitations of strongly correlated systems. In this talk, a theoretical (diagrammatic) framework of the linear response of LDA+U (TDLDA+U) functional will be presented and applied to the study of Frenkel excitons in NIO within the first-principles Wannier basis. The advantages and disadvantages of LDA+U functional will be discussed, in comparison with more advanced many-body approaches. [1] B. C. Larson, et al. PRL 99, 026401 (2007)*Work supported by U.S. DOE - CSMN

11:39AM V13.00003 Propagation of strongly bound Frenkel excitons in LiF: An effective two-particle kinematic approach of super-atom in ab initio Wannier basis1, CHEN-LIN YEH, HUNG-CHUNG HSUEH, Department of Physics, Tamkang University, Taiwan, WEI KU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, NY, USA — A general new first-principles Wannier function based method is proposed to better understand the propagation of strongly bound Frenkel excitons. Specifically, long-standing debate of the Frenkel nature of the excitons in LiF is made apparent by the formation of a “super-atom” consisting of Wannier orbitals from both Li and F. On this basis, a new approach is proposed by formulating the kinematic contribution to the propagation of the exciton via an effective two-particle hopping kernel. The same kernel contains both the mass enhancement at strong binding and the decay into continuum at weak binding, and is thus exact in both limits. This kinematic effect is compared with found to overwhelm the conventional interaction-based propagations of exciton in LiF. This general theoretical framework can be directly applied to the study of propagation of local excitations of strongly correlated systems.

1National Science Council No. 106, HoPing E. Road, Sec.2, Taipei 10622, Taiwan (R.O.C.)

11:51AM V13.00004 Ab-initio Total Energy Calculation for Full-potential Multiple Scattering Theory Methods1, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, AURELIAN RUSANU, MALCOLM STOKES, DON NICHOLSON, MARKUS EISENBACK, Oak Ridge National Laboratory — The ab initio methods (e.g., KKR, KKR-CPA, LSMS) based on multiple scattering theory have the clear advantage of being able to calculate the Green function in a straightforward manner, which has important implications in the application of electronic structure calculations. But these methods have mostly been implemented within muffin-tin approximations. Recent advances in the numerical implementation of full-potential multiple scattering theory and, in particular, the development of an innovative Poisson equation solver have made carrying out the fully self-consistent full-potential calculation possible. In this presentation, we discuss various implementations of the full-potential total energy calculation, and we investigate the convergence of the total energy with respect to the angular momentum expansion cutoff for scattering matrices. Finally, we compare the full-potential total energy with the muffin-tin approximation results.

1This work is supported by US-DOE, Office of Basic Energy, Division of Materials Science and Engineering.

12:03PM V13.00005 A quantum chemistry roadmap towards highly accurate adsorption energies at ionic surfaces, BO LI, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ANGELOS MICHAELIDES, London Centre for Nanotechnology, University College London and Fritz-Haber-Institut der Max-Planck-Gesellschaft, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft — A roadmap is established to compute adsorption energies of molecules at ionic surfaces with an accuracy approaching chemical accuracy (a precision of 1 kcal/mol or ~43 meV). The approach relies on established quantum chemistry methodologies and involves a separation of the total adsorption energy into contributions from Hartree-Fock and electron correlation, the use of embedded cluster models of the substrate, and extrapolations to the complete basis set limit. Application of the procedure to the example of water on salt, with electron correlation treated at the CCSD(T) level, yields an adsorption energy for a water monomer on NaCl(001) of 480 ± 20 meV.
12:15PM V13.00006 Surface energies of semiconductors by the energy density method. MIN YU, RICHARD M. MARTIN — Energy Density formalism within the first-principles pseudopotential density functional theory has been proposed by Chetty and Martin in 1990s. Although the energy density function is non-unique, nevertheless integrals over surface regions provide unique results for surface energies, and calculations have been carried out by several groups to study the polar surfaces and interfaces of solid state systems such as GaAs (111) and (111) polar surfaces. In our work, we apply this method to wurtzite CdSe to determine the energy of various polar surfaces such as (0001), (0001), and non-polar surfaces such as (1010), (1120), from which we can estimate the equilibrium crystal shape for large nanoclusters. 1. N. Chetty and Richard M. Martin, Phys. Rev. B 45, 6074 (1992). 2. K. Rapcewicz, B. Chen, B. Yakobson, and J. Bernholc, Phys. Rev. B 57, 7281 (1998). 3. N. Moll, A. Kley, E. Pehlke, and M. Scheffler, Phys. Rev. B 54, 8844 (1996).

12:27PM V13.00007 Electron-phonon interaction using Wannier functions: from single-layer graphene to cuprate superconductors. FELICIANO GIUSTINO, Department of Physics, University of California at Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — The interaction between electrons and phonons is central to many phenomena, including electrical and thermal transport and superconductivity. Recently the electron-phonon (e-ph) interaction has been the focus of intense research efforts in the physics of high-temperature superconductivity and nanoscale transport. Despite the continued interest in the e-ph problem, first-principles calculations remain challenging due to the large computational effort required to describe e-ph scattering processes in the proximity of the Fermi surface. In this talk I will present a method based on Wannier functions which greatly reduces the computational cost of e-ph calculations [1,2]. The underlying idea is to exploit the spatial localization of electrons, and phonons in the maximally localized Wannier representation. After describing the method I will review recent applications to materials of current interest. I will discuss how the e-ph interaction affects the dynamics of Dirac fermions in graphene [3], the origin of superconductivity in boron-doped diamond [4], and the relation between Fermi surface topology and superconductivity in super-hard carbides. I will conclude this presentation by discussing the role of phonons in the angle-resolved photoemission spectra of cuprates [4].

1 Supported by NSF grant CHE-0304710.

1:03PM V13.00008 Ensemble density functional theory, the atom-in-molecule problem, and reactive charge transfer. SUSAN ATLAS, Department of Physics and Astronomy, University of New Mexico, STEVEN VALONE, Materials Science and Technology Division, Los Alamos National Laboratory — A major challenge in large-scale simulations of complex biomolecular and materials systems is the ability to accurately describe reactive dynamics. We have previously described a new multiscale formalism, based on density functional theory and the embedded-atom method, that enables the rigorous encoding of quantum mechanical excitation effects such as charge polarization and charge transfer within a classical potential. Here we describe a new formulation of a key element of the theory: the deconstruction of molecular densities into subsystem atom-in-molecule components via ensemble constrained-search density functional theory. The method is implemented via the self-consistent solution of coupled sets of Kohn-Sham equations in conjunction with chemical potential equalization across subsystems. This leads to a natural interpretation of dynamical charge transfer and charge polarization in terms of an electronic entropy, thus extending the seminal work of Gross, Oliveira, and Kohn (1988).

1:15PM V13.00009 Correction of Finite Size Errors in Many-body Electronic Structure Calculations. HENDRA KWEE, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — Finite-size (FS) effects are a major source of error in many-body (MB) electronic structure calculations of extended systems. Reducing FS errors is thus a key to broader applications of MB methods in real materials, and the subject has drawn considerable attention. We show that MB FS effects can be effectively included in a modified local density approximation calculation. A parametrization for the FS exchange-correlation functional is obtained. The method is simple and gives post-processing corrections that can be applied to any MB results. Conceptually, it gives a consistent framework for relating FS effects in MB and DFT calculations, which is important if the two methods are to be seamlessly interfaced to bridge length scales. Applications to a model insulator (P₂ in a supercell), to semiconducting Si, and to metallic Na show that the method delivers greatly improved FS corrections.

1 Supported by ONR, NSF, and ARO.

1:27PM V13.00010 Embedding quantum-mechanics in an interatomic potential simulation using local energies. NOAM BERNSTEIN, Naval Research Laboratory, GABOR CSANYI, University of Cambridge — Atomistic simulations that use quantum-mechanical total-energy models provide high accuracy and reliability at the price of computational expense. Classical approximations such as interatomic potentials are much faster, but less transferable. We couple the two approaches concurrently, to describe part of the system quantum-mechanically and part with interatomic potentials, using a weighted sum of atomic energies. This enables us to compute a well defined total energy and part with interatomic potentials, using a weighted sum of atomic energies. The underlying idea is to exploit the spatial localization of electrons, and phonons in the maximally localized Wannier representation. After describing the method I will review recent applications to materials of current interest. I will discuss how the e-ph interaction affects the dynamics of Dirac fermions in graphene [3], the origin of superconductivity in boron-doped diamond [4], and the relation between Fermi surface topology and superconductivity in super-hard carbides. I will conclude this presentation by discussing the role of phonons in the angle-resolved photoemission spectra of cuprates [4].

1 Funded by DOE-SC-BES-DM.
Using genetic algorithms to find from first-principles the minimum-energy crystal structure starting from random cell vectors and random atomic positions.\(^1\) G. TRIMARCHI, M. D’AVEZAC, ALEX ZUNGER, NREL, Golden CO 80401 — We address the global space-group optimization problem in binary metallic \(A_2B_1\)\(_\text{x} \)\(-\text{y}\)\(_\text{z}\) alloys using an evolutionary algorithm. A set of crystal structures with randomly-chosen lattice vectors and atomic positions is evolved, replacing the highest energy structures with new ones generated through mating or mutation, as well as ab-initio structural relaxation to the nearest local minimum. This was applied to a few compounds whose lattice-type is difficult to guess because the constituent solids \(A\) and \(B\) have different lattice types (e.g., \(A\) is fcc and \(B\) is bcc): (i) compounds with the crystal lattice of either \(A\) or \(B\) constituents, i.e., \(\text{CdPt}_3\), \(\text{AlSc}_3\), \(\text{Al}_5\text{Sc}\); (ii) compounds with a crystal lattice different than that of either constituents, i.e., \(\text{AlSc}\) and \(\text{CuPd}\); (iii) compounds whose crystal lattice is not even of a Bravais type, e.g., \(\text{PdTi}_2\). The optimization scheme retrieved the lowest energy structures within about 100 total-energy evaluations. Not all independent \(GA\) sequences end up giving the same final structure; we select the lowest energy structure from all sequences. Using a model calculation, we will discuss how many independent \(GA\) sequences are needed to find the lowest energy structure with given confidence.

\(^1\) Funded by DOE-SC-BES-DMS

From grand-canonical density functional theory towards rational compound design, ANATOLE VON LILIENFELD, Sandia National Laboratories — The fundamental challenge of rational compound design, i.e., the reverse engineering of chemical compounds with predefined specific properties, originates in the high-dimensional combinatorial nature of chemical space. Chemical space is the hyper-space of a given set of molecular observables that is spanned by the grand-canonical variables (particle densities of electrons and nuclei) which define chemical composition. A brief but rigorous description of chemical space within the molecular grand-canonical ensemble multi-component density functional theory framework will be given \([1]\). Numerical results will be presented for intermolecular energies as a continuous function of alchemical variations within a neutral and isoelectronic 10 proton system, including \(\text{CH}_4\), \(\text{NH}_3\), \(\text{H}_2\text{O}\), and HF, interacting with formic acid \([2]\). Furthermore, engineering the Fermi level through alchemical generation of boron-nitrogen doped mutants of benzene shall be discussed \([3]\).

\(^1\) von Liliendel and Tuckerman JCP 125 154104 (2006)
\(^2\) von Liliendel and Tuckerman JCTC 3 1083 (2007)
\(^3\) Marcon et al. JCP 127 064305 (2007)

**Thursday, March 13, 2008 11:15AM - 1:51PM**

Session V14 DAMOP: BEC-BCS Crossover Morial Convention Center 205

Properties of a few-body trapped two-component Fermi gas at unitarity\(^1\), JAVIER VON STECHER, Department of Physics and JILA, University of Colorado, Boulder, CO 80309-0440, DOERTE BLUME, Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, CHRIS H. GREENE, Department of Physics and JILA, University of Colorado, Boulder, CO 80309-0440 — We consider a trapped two-component Fermi system with even and odd number of fermions \(N\). Unlike fermions interact with a short-range two-body potential which does not support a bound state and is characterized by an infinite scattering length. Using two different numerical techniques, i.e., a correlated Gaussians basis expansion method and a fixed-node diffusion Monte Carlo method, we solve the many-body Schrodinger equation and determine the spectrum and structural properties. Analyzing the excitation spectrum and the wavefunctions, we demonstrate that this system exhibits unique universal properties \([1]\), in agreement with analytical predictions \([2]\). Furthermore, we determine the excitation gap up to \(N = 30\) and we compare it with recent predictions. \([1]\) D. Blume, J. von Stecher, and Chris H. Greene, e-print arXiv:cond-mat/0708.2734 \([2]\) F. Werner and Y. Castin, Phys. Rev. A 74, 053604 (2006).

\(^1\) This work was supported in part by NSF.

Quantum and thermal fluctuations in the BCS-BEC crossover with unequal mass fermions, ROBERTO DIENER, QI ZHOU, MOHIT RANDERIA, The Ohio State University — A lot of progress has been done in the study of the BCS-BEC crossover for equal-mass fermions in recent years by both theory and experimental groups. An extension of this problem which is starting to receive more attention is the study of mixtures of fermions with different masses, such as a mixture of \(^{40}\)K and \(^{6}\)Li. Using our functional integral method, which we have previously used to study the equal-mass case and which includes the effect of collective excitations \([1]\), we have studied the properties of a fermionic gas with unequal masses across the BCS-BEC crossover. We will present results for different thermodynamical quantities as a function of mass ratio and interaction strength: e.g., the beta parameter at unitarity, the ground state energy as a function of \(1/(k_F \alpha)\), as well as the dimer scattering in the BEC limit as a function of mass ratio which agrees to within 20% with the exact four-body calculation of D. Petrov et al., J. Phys. B At. Mol. Opt. Phys. 38, S645 (2005).

Critical temperature and thermodynamics of the BEC-BCS crossover, EVGENI BUROVSKI, Uni Greifswald, Germany, EVGENY KOZIK,NIKOLAY PROKOF’EV, BORIS SVISTUNOV, UMASS Amherst, MATTHIAS TROYER, ETH Zurich — The strongly-correlated regime of the BCS-BEC crossover can be realized by diluting a system of two-component fermions with a contact attractive interaction and an appropriate ultraviolet regularization. We investigate this system via a novel systematic-error-free continuous-space-time diagrammatic determinant Monte Carlo method. The results allow us to predict the universal curve \(T_c/E_F\) as a function of the parameter \(k_F \alpha\) with the maximum on the BEC side. At unitarity, \(T_c/E_F = 0.152(7)\). We also determine the thermodynamic functions and show how the Monte Carlo results can be used for accurate thermometry.

First- and second-sound-like modes at finite temperature in trapped Fermi gases from BCS to BEC, YAN HE, CHIH-CHUN CHIEN, QIJIN CHEN, KATHRYN LEVIN, University of Chicago — We determine the temperature \((T)\) dependence of first- and second-sound frequency modes for trapped Fermi gases undergoing the BCS to Bose-Einstein condensation (BEC) crossover. Our results are based on numerical solution of the two-fluid equations in conjunction with a microscopic calculation of thermodynamical variables. As in experiment and at unitarity, we show that the lowest radial breathing mode is \(T\) independent. At finite \(T\), higher-order breathing modes strongly mix with second sound. Their complex \(T\) dependence should provide an alternative way of measuring the transition temperature \(T_c\). We will also discuss collective mode frequency for polarized Fermi gas.
12:03PM V14.00005 Transport Properties of a Fermi gas with attractive interactions in the BEC-BCS crossover. CHIH-CHUN CHIEN, YAN HE, QIYUN CHEN, KATHRYN LEVIN, University of Chicago — The transport phenomena of a two-component Fermi gas with attractive interactions are studied at finite temperatures focused on the normal state using a t-matrix formalism in the BEC-BCS crossover. We contrast the behavior of both charged and uncharged systems and address such varied coefficients as DC conductivity and shear viscosity. We show how the behavior above the pairing onset temperature $T^*$ appears to depend rather weakly on the scattering length. At lower temperatures by studying the appropriate Maki–Thompson and Aslamazov-Larkin diagrams, we find more pronounced fluctuation effects the closer the system is to the BCS limit. Interestingly, we observe that these fluctuation effects are more charged than in uncharged systems.

12:15PM V14.00006 Probing two-fluid hydrodynamics in a trapped Fermi superfluid at unitarity1, EDWARD TAYLOR2. ALLAN GRIFFIN, University of Toronto, HUI HU3, XIA-JI LIU, University of Queensland — We develop a variational approach to calculate the density response function at finite temperatures of the lowest-lying two-fluid dipole and breathing modes in a trapped two-component Fermi superfluid close to a Feshbach resonance. The out-of-phase oscillations, which are the analogue in trapped gases of second sound in uniform superfluids, have so far not been observed in cold-atom experiments. At unitarity, we show that these modes are observable at finite temperatures via two-photon Bragg scattering, whose spectrum is related to the imaginary part of density response function. This provides direct evidence for superfluidity and a promising way to test microscopic results for thermodynamics at unitarity. (arXiv:0709.0698, 0711.0561).

12:27PM V14.00007 Shear Viscosity and the Perfectness of Fluid. GAUTAM RUPAK, THOMAS SCHAFFER, North Carolina State University — A recent calculation of the shear viscosity for a unitary gas is presented. Here unitary gas is defined as a non-relativistic Fermi gas with infinite scattering length. The unitary gas is a scale invariant strongly-interacting many-body system, and possesses universal properties that are of interest across subfields in physics. A unitary gas can be realized in cold atomic gas experiments near a Feshbach resonance. Conditions approximating the unitary gas emerge in low energy nuclear physics as well. From general principle, the shear viscosity of a strongly interacting gas should be small, however, quantum mechanics places a lower bound. A strict lower bound indicating how “perfect” a fluid can become has been conjectured from calculations in strongly coupled field theories that have a gravity dual. We test this conjecture with an explicit calculation in a unitary gas, the most strongly interacting non-relativistic system experimentally known.

12:39PM V14.00008 Spectroscopic Signatures of Nonequilibrium Pairing in Atomic Fermi Gases1, MAXIM DZERO, Columbia University, EMIL YUZBASHYAN, Rutgers University, B.L. ALTSHULER, Columbia University, PIERS COLEMAN, Rutgers University — We present the results of a theoretical description of the radio-frequency (RF) spectra for non-stationary states of a fermionic condensate. These states can be produced by a rapid switch of the scattering length. We show that the RF spectrum of the nonequilibrium state with constant BCS order parameter has two features in contrast to equilibrium where there is a single peak. The additional feature reflects the presence of excited pairs in the steady state. In the state characterized by periodically oscillating order parameter RF-absorption spectrum contains two sequences of peaks spaced by the frequency of oscillations. Satellite peaks appear due to a process where an RF photon in addition to breaking a pair emits/absorbs oscillation quanta.

The work of M. D. and P. C. was supported by the DOE Grant No. DOE-DE02-00ER45790. E.Y. was supported by the Alfred P. Sloan Foundation and NSF Grant No. NSF-DMR-0547769.

12:51PM V14.00009 Mean Frequency Shift and Finite Width of RF Spectrum of Paired Fermions, ZHENHUA YU, Department of Physics, University of Illinois, 1110 W. Green Street, Urbana, IL 61801 — Using sum rules we derived the mean frequency shift of the rf spectrum of paired fermions in terms of the derivative of free energy, and explained many features of experiments done at the unitarity point between the lowest hyperfine states of $^6$Li. The calculated mean shifts are however some three times larger than the peak shift observed at the center of the trapped atomic cloud, a discrepancy due to the long tail of the spectrum. Generating the rf spectrum function self-consistently within BCS-Hartree-Fock, we have determined the characteristic frequency where the behavior of the spectrum transits from $\omega^{-3/2}$ to $\omega^{-5/2}$ at large frequency. We discuss how to subtract out the long tail from the spectrum and give an improved estimate for the peak frequency shift from the sum rules.


1:03PM V14.00010 Final-state effects in radio-frequency spectrum of ultracold Fermions, SOURISH BASU, ERICH MUELLER, Cornell University — We model the effects of final-state interaction on the radio-frequency spectrum of a two-component superfluid Fermi gas near resonance. We show how the spectrum evolves as one tunes from weak to strong interactions. Aside from the continuum resulting from the breaking of Cooper pairs, for certain interaction strengths, we predict a sharp peak resulting from converting a pair in one channel to a pair in another channel.

1:15PM V14.00011 Molecular production at a broad Feshbach resonance in Fermi-gas of cooled atoms, DEQIANG SUN, ARTEM ABANOV, VALERY POKROVSKY, Texas A&M University — The problem of molecular production from a degenerate gas of fermions at a broad Feshbach resonance, in a single-mode approximation, is reduced to the linear Landau-Zener problem for operators. The strong interaction leads to significant renormalization of the gap between adiabatic levels. In contrast to the static problem, the close vicinity of the exact resonance does not play a substantial role. The two main physical results are: i) The molecular production is sensitive to the initial magnetic field. ii) In the inverse process of molecule dissociation a large BCS condensate distributed over a broad range of momenta is generated.

1:27PM V14.00012 Bistability in Resonant Fermi Superfluid1, LEI JIANG, HAN PU, Rice University, ANDREW ROBERTSON, HONG LING, Rowan University — The resonant two-channel Fermi superfluid model can be mapped to a quantum optics model that describes a single-mode laser field, subject to Kerr nonlinearity, interacting with an ensemble of inhomogeneously broadened two-level atoms. Using this analogy, we show that under proper conditions bistability will occur in resonant Fermi superfluids, a matter wave analog of a similar phenomenon encountered in nonlinear optical systems.

1This work is supported by NSF, ARO and the Welch Foundation.
1:39PM V14.00013 Collective spin modes in a Fermionic atomic gas , JOHN FELDMANN, HARI DAHAL, Boston College, SERGIO GAUDIO, University of Rome La Sapienza, KEVIN BEDELL, Boston College — We present our theoretical findings on the structure of the spin mode dispersion of a spin-population-imbalanced Fermionic atomic gas in the highly degenerate regime, but above the superfluid critical temperature, near a Feshbach resonance. We employ standard Fermi liquid theory to describe a gas consisting of two species of spin, up and down, existing in an external magnetic field, which models an atom gas of $^6$Li atoms in the two lowest Zeeman states. The spin population imbalance creates a net magnetization, and as a result, the transverse magnetization propagates through the system. We find that a diverging scattering length, as occurs near a Feshbach resonance, affects the phenomenological Landau parameters of the system, whose relation to the scattering length is described by the induced interaction model, and thus in turn affects the structure of the collective spin modes, as well.


11:15AM V15.00001 The structure of preserved information in quantum processes , HUI KHOONG NG, Caltech, ROBIN BLUME-KOHOUT, Perimeter Institute, DAVID POULIN, Caltech, LORENZA VIOLA, Dartmouth College — We present a general operational framework for characterizing the types of information that can be preserved by a quantum process. We demonstrate that information preserving structures (IPS) – encompassing noiseless subsystems, decoherence-free subspaces, pointer bases, and error-correcting codes – are isometric to fixed points of unital quantum processes. This implies that every IPS is a matrix algebra. A structure theorem for fixed points of an arbitrary process further provides a simple and efficient algorithm for finding all noiseless and unitarily noiseless IPS for any quantum process. This framework can be extended to study the structure of approximately preserved information.

11:27AM V15.00002 Decoherence-free subspaces and incoherently generated coherences, RAISA KARASKI, BQIC and Applied Science & Technology, University of California, Berkeley, KARL-PETER MARZLIN, BARRY C. SANDERS, IQIS, University of Calgary, KIRIGITTA WHALEY, BQIC and Dept. of Chemistry, University of California, Berkeley — A decoherence-free subspace (DFS) is a collection of states that is immune to the dominant noise effects created by the environment. DFS is usually studied for states involving two or more particles and is considered a prominent candidate for quantum memory and quantum information processing. We present rigorous criteria for the existence of DFS in finite-dimensional systems coupled to the Markovian reservoirs. This allows us to identify a new special class of decoherence-free states that relies on rather counterintuitive phenomenon, which we call an “incoherent generation of coherences.” We provide examples of physical systems that support such states.

11:39AM V15.00003 Methods for Producing Decoherence-free States and Noiseless Subsystems Using Photonic Qutrits, C. ALLEN BISHOP, MARK BYRD, Physics Department, Southern Illinois University Carbondale — We outline a proposal for a method of preparing a single logically encoded two-stage system (qubit) that is immune to collective noise acting on the Hilbert space of the particles supporting it. The logical qubit is comprised of three photonic 3-state systems (qutrits) and is generated by the process of spontaneous parametric downconversion. The states are constructed using linear optical elements along with three down-conversion sources, and are deemed successful by the simultaneous detection of six events. We also show how to select a maximally entangled state of two qutrits by similar methods. For this maximally entangled state we describe conditions for the state to be decoherence-free which do not correspond to collective errors, but which have a precisely defined relationship between them.

1Supported by the NSF through grant No. 0545798 to MSB.

11:51AM V15.00004 Bounded-strength dynamical control of qubit coherence based on Eulerian cycles, LEA F. SANTOS, Yeshiva University, TAYLOR S. SMITH, WENXIAN ZHANG, LORENZA VIOLA, Dartmouth College — Decoherence and faulty controls are two of the primary obstacles to realize scalable quantum information processing. Here, we investigate dynamical decoupling (DD) techniques for dynamical control and decoherence suppression in the limit of low-power faulty control, using the approach of Eulerian DD introduced in L. Viola and E. Knill, Phys. Rev. Lett. 90, 037901 (2003). By focusing on the illustrative case of single-qubit DD, we identify scenarios where naive transcriptions of bang-bang sequences with finite pulses are outperformed by the Eulerian method – both in terms of DD fidelity and robustness against systematic errors. Results on Eulerian decoherence control in solid-state qubit devices are presented.

1Supported in part by the NSF through grant No. PHY-0555417 and by the DOE through contract No. DE-AC02-07CH11358.

12:03PM V15.00005 Model-independent dynamical decoupling to combat dephasing decoherence, WAYNE WITZEL, BENJAMIN LEE, SANKAR DAS SARMA, University of Maryland, College Park — We present a remarkable finding that a recently [1] discovered series of pulse sequences, designed to optimally restore coherence to a qubit in the spin-boson model of decoherence, is in fact completely model-independent and generically valid for arbitrary dephasing Hamiltonians given sufficiently short delay times between pulses [2]. The series is optimal in that fidelity is maximized for a given number of applied pulses. This is true for sufficiently short delay times because the series, with each pulse, cancels successive orders of a time expansion for the decay of qubit fidelity. Surprisingly, this property is independent of the model of the bath that induces dephasing-type decoherence. For this to be true, a linearly growing set of “unknowns” (the delay times) simultaneously satisfy an exponentially growing set of non-linear equations. This is an unexpected and miraculous property of nature and mathematics. [1] G. S. Uhrig, Phys. Rev. Lett. 98, 100504 (2007). [2] B. Lee, W. M. Witzel, S. Das Sarma, arXiv:0710.1416.

1Supported by LPS-NSA and ARO-DTO.
2Naval Research Laboratory
3Magnet Program, Montgomery Blair High School, Silver Spring, MD

12:15PM V15.00006 Encoding One Logical Qubit Into Six Physical Qubits, BILAL SHAW, MARK WILDE, OGNYAN ORESHKOV, ISAAC KREMSKY, DANIEL LIDAR, University of Southern California — We discuss several methods to protect one qubit against single-qubit errors by encoding it into six physical qubits. We first present a degenerate six-qubit quantum error-correcting code. We explicitly provide the stabilizer generators, encoding circuit, codewords, logical Pauli operators, and logical CNOT operator for this code. We then prove that a six-qubit code cannot simultaneously possess a Calderbank-Shor-Steane stabilizer and correct arbitrary single-qubit errors. We finally construct a six-qubit non-degenerate entanglement-assisted quantum error-correcting code that uses one bit of entanglement shared between the sender and the receiver. We discuss the advantages and disadvantages for each of our six-qubit quantum error-correcting codes.
12:27PM V15.00007 Second-order self-refocusing pulse shapes for arbitrary rotation angles, LEONID P. PRYADKO, University of California, Riverside, PINAKI SENGUPTA, Los Alamos National Laboratory — We construct several families of high-precision 1st- and 2nd-order self-refocusing pulse shapes for rotation angles $\alpha = 0^\circ, 10^\circ, \ldots, 360^\circ$. To characterize their performance, we show that for an arbitrarily-coupled qubit driven by a general one-dimensional symmetric pulse shape, in addition to the net rotation angle, the second-order average Hamiltonian is defined by three parameters. Our 1st- and 2nd-order self-refocusing pulses respectively have one or two of these equal to zero, which makes them useful as a drop-in replacement for hard pulses. We illustrate this by analyzing several commonly-used composite pulses in terms of the average Hamiltonian theory. The results are in an excellent agreement with numerical simulations.

1This research was supported in part by the NSF grant No. 0622242 (LP)

12:39PM V15.00008 Encoded Dynamical Recoupling with Shaped Pulses, YUNFAN LI, University of California, Riverside, DANIEL A. LIDAR, University of Southern California, LEONID P. PRYADKO, University of California, Riverside — Encoded Dynamical Recoupling is a passive error correction technique which can be used to enhance the performance of a quantum error correction code (QECC) against low-frequency component of the thermal bath. The elements of the stabilizer group are used in the decoupling cycle which makes the encoded logic operations fault-tolerant. We studied the effectiveness of this technique both analytically and numerically for several three- and five-qubit codes, with decoupling sequences utilizing either Gaussian or self-refocusing pulse shapes. When logic pulses are intercalated between the decoupling cycles, the technique may be very effective in cancelling constant perturbation terms, but its performance is much weaker against a time-dependent perturbation simulated as a classical correlated noise. The decoupling accuracy can be substantially improved if logic is applied slowly and concurrently with the decoupling, so that a certain adiabaticity condition is satisfied.

12:51PM V15.00009 Generating Novel Spin Echoes Using the Internal Structure of Strong Pi-Pulses, YANQUN DONG, RONA RAMOS, DALE LI, SEAN BARRETT, Yale University — Conventionally, strong pulses used to control coherent evolution are approximated as instantaneous, perfect rotations. However, recent experiments have shown a surprising departure from the conventional theory in standard multipulse NMR experiments using strong pi-pulses. Using our understanding of the role that the finite time duration of any real pulse plays in these effects, we design and experimentally demonstrate new classes of spin echoes.

1:03PM V15.00010 A New Approach to Spin Coherence Control: Extreme Line-narrowing and MRI of Solids, YANQUN DONG, RONA RAMOS, DALE LI, SEAN BARRETT, Yale University — The non-zero duration of strong pulses has been shown to have surprisingly large effects in important NMR experiments. The Hamiltonian terms arising from the internal structure of strong pulses provide us with a new technique of spin coherence control. Using this technique, we design and demonstrate new approaches to line-narrowing and magnetic resonance imaging of solids.

1:15PM V15.00011 Robustness of operator quantum error correction against imperfect initialization, OGVYAN ORESHKOV, University of Southern California — It is known that perfect unitary evolution inside decoherence-free subspaces and line-narrowing and magnetic resonance imaging of solids. Also, we present a scheme for performing state preparation, which is the mapping a fiducial state to an arbitrary target state, and show simulations that drop-in replacement for hard pulses. We illustrate this by analyzing several commonly-used composite pulses in terms of the average Hamiltonian theory. The results are in an excellent agreement with numerical simulations.

1:27PM V15.00012 Quantum Convolutional Coding with Entanglement Assistance, MARK WILDE, TODD BRUN, University of Southern California — We have recently developed quantum convolutional coding techniques for both entanglement distillation and quantum error correction. These techniques assume that the two parties participating in the communication protocols possess prior shared entanglement. Using these methods, we can import arbitrary classical binary or quaternary convolutional codes for use in quantum coding, with no requirement that these codes be self-orthogonal. Moreover, high-performance classical convolutional codes lead to high-performance quantum convolutional codes. We explicitly show how a convolutional entanglement distillation protocol operates, and how to encode and decode a stream of quantum information in an entanglement-assisted quantum convolutional code.

1Support from NSF Grants CCF-0545845 and CCF-0448658.

1:39PM V15.00013 “Slow” and “Fast” Gate Limits In Resilient Quantum Computation, EDUARDO NOVAIS, Duke University, EDUARDO R. MUCCHIOLO, University of Central Florida, HAROLD U. BARANGER, baranger@phy.duke.edu — In the study of resilient quantum computation, there are two common approaches to proving the threshold theorem: one either uses a stochastic error model or uses the operator norm to bound the effects of the noise. In many cases, the underlying microscopic Hamiltonian is hidden due to the rapidly growing complexity of the problem. In particular, the microscopic interacting Hamiltonian in the interaction picture depends on the quantum code and its implementation. Nevertheless, there are two possible ways to keep the discussion code independent. The first situation is to imagine very fast gates acting on the system. The second is to derive an upper bound on the effects of correlations by deriving an effective model. In this talk we discuss these two limits, focusing on how to derive the effective model for “slow gates”.

1This work was supported in part by NSF grants No. CCF 0523509 and No. CCF 0523603. E.R.M. acknowledges partial support from the Interdisciplinary Information Science and Technology Laboratory (12Lab) at UCF.

1:51PM V15.00014 Optimal Control of Large Spin-Atomic Systems with Coherent Electromagnetic Fields, SETH MERKEL, University of New Mexico, SOUMA CHAUDHURY, POUL JESSEN, University of Arizona, IVAN DEUTSCH, University of New Mexico — Cold atomic systems provide an excellent testing ground for quantum control protocols due to the isolation of these systems from their environment and the availability of high precision fields from the “quantum optics toolbox”. In this talk, we look at controlling the sixteen dimensional ground state hyperfine manifold of $^{133}\text{Cs}$ through microwaves and rf-magnetic fields. These controls allow for essentially coherent manipulation of a system that is large enough to exhibit non-trivial dynamics. In particular, we analyze the controllability of this system under different combinations of applied electromagnetic fields. Also, we present a scheme for performing state preparation, which is the mapping a fiducial state to an arbitrary target state, and show simulations that examine the performance of these state preparation protocols.

1This research was supported by NSF Grants No. PHY-0355073 and No. PHY-0355040, ONR Grant No. N00014-05-1-420, and DTO Grant No. DAAD19-13-R-0011.
2:03PM V15.00015 Towards a Quantum Predictive Control Mathematical Formulation, YASSER A. DAVIZON-CASTILLO, Department of Electrical Engineering, Arizona State University — Quantum Feedback Control presents an interdisciplinary research work between Control Theory and Quantum Physics. A novel mathematical formulation is presented for Quantum Predictive Control (QPC) algorithm, based on Receding Horizon Control philosophy at the quantum level. The application of Heisenberg Uncertainty Principle, to quantify the uncertainty in position and momentum, in a real-time control framework is introduced. An estimate of the Sampling Time at quantum level is demonstrated, applying to a case of study for a double well quantum system using the QPC algorithm.

Thursday, March 13, 2008 11:15AM - 2:15PM —
Session V16 DBP: Focus Session: Medical Imaging and Related Technologies Morial Convention Center 208

11:15AM V16.00001 Overview of Medical Imaging, WILLIAM HENDEE, Medical College of Wisconsin — The use of radiation probes to image tissues in the human body has progressed through an extraordinary evolution in the past three decades. Beginning with transmission computed tomography in the 1970s, this evolution has included real-time ultrasound, emission computed tomography, magnetic resonance imaging, and digital radiography. These advances have recently yielded major improvements in imaging such as multi-detector transmission computed tomography, functional magnetic resonance imaging, dual imaging modalities built on a common platform, and image-guided intervention. These improvements and others have accelerated the usefulness of imaging methods in the early detection, definitive diagnosis, and effective intervention of a wide spectrum of diseases and disabilities. They also have led to increases in radiation doses to patients and the population, an issue of major concern to physicists and physicians. At this time there are four major frontiers for research in medical imaging: (1) molecular imaging; (2) functional imaging; (3) multi-modality imaging; and (4) information management. These research frontiers, together with the use of sophisticated imaging technologies in clinical practice, offer rich professional opportunities for physicists.

11:51AM V16.00002 PET Imaging - from Physics to Clinical Molecular Imaging, STAN MAJIEWSKI, Thomas Jefferson National Accelerator Facility — From the beginnings many years ago in a few physics laboratories and first applications as a research brain function imager, PET became lately a leading molecular imaging modality used in diagnosis, staging and therapy monitoring of cancer, as well as has increased use in assessment of brain function (early diagnosis of Alzheimer’s, etc) and in cardiac function. To assist with anatomic structure map and with absorption correction CT is often used with PET in a duo system. Growing interest in the last 5-10 years in dedicated organ specific PET imagers (breast, prostate, brain, etc) presents again an opportunity to the particle physics instrumentation community to contribute to the important field of medical imaging. In addition to the bulky standard ring structures, compact, economical and high performance mobile imagers are being proposed and build. The latest development in standard PET imaging is introduction of the well known TOF concept enabling clearer tomographic pictures of the patient organs. Development and availability of novel photodetectors such as Silicon PMT immune to magnetic fields offers an exciting opportunity to use PET in conjunction with MRI and fMRI. As before with avalanche photodiodes, particle physics community plays a leading role in developing these devices. The presentation will mostly focus on present and future opportunities for better PET designs based on new technologies and methods: new scintillators, photodetectors, readout, software.

12:27PM V16.00003 Room temperature STM imaging in air can damage DNA, even at low tunneling biases and currents1, JOHN BECHHOEFER, PHILIP GRANT, YUEKAN JIAO2, Simon Fraser University — STM images of DNA molecules in air or vacuum at room temperature have been plagued by problems of reproducibility. These difficulties have usually been ascribed to substrate artifacts or tip-related effects. However, the recent discovery that low-energy electron beams cause single-strand breaks in DNA suggests that the tunneling electrons used for STM imaging can damage DNA similarly and could be responsible for many imaging problems. Here, we provide experimental support for such a conclusion. Collecting images from an STM that simultaneously detects light-emission from the tip region, we show that the observed DNA structure changes after the first scan. The organic debris from the DNA quenches the light emission from surface plasmons on the gold substrate. Next, we use an atomic force microscope (AFM) whose stiff tip can be used both for tapping-mode AFM and for STM imaging modes. We assess STM-induced damage by re-imaging the same area in tapping-mode AFM. The bias-dependent change in DNA film thickness correlates with the previously observed rate of DNA strand breaks caused by low-energy electron beams of different energies.

1:03PM V16.00006 Advances in Medical X-Ray Imaging, ROBERT GOULD, University of California San Francisco — No abstract available.

1:22PM V15.00011 Imaging of biological interfaces at the nanoscale, OSCAR MESQUITA, Physics Department, Federal University of Minas Gerais — Transparent objects can render visible in a standard bright-field microscope by slightly defocusing the microscope objective. From contrast fluctuations of images defocused in a controlled way one can measure the fluctuation spectrum of biological membranes and living cells surfaces. We extended our previous defocusing theory, valid for small defocusings, to arbitrarily large defocusings. We discovered that we can measure height fluctuations of transparent interfaces selectively, and obtain elastic properties of layered biological membranes separately. As an example, we measured separately the elastic constants associated with the two opposite surfaces of a red blood cell. The technique is very sensitive and allows us to measure the small increase of surface tension on the surface in contact with the glass-slide, as compared to the one of the free surface. Interface roughness (static and dynamic), down to nanometer amplitudes, can be measured selectively with defocusing microscopy in transparent layered materials.

12:39PM V16.00004 Tomography of biological interfaces using defocusing microscopy, OSCAR MESQUITA, Physics Department, Federal University of Minas Gerais — Transparent objects can render visible in a standard bright-field microscope by slightly defocusing the microscope objective. From contrast fluctuations of images defocused in a controlled way one can measure the fluctuation spectrum of biological membranes and living cells surfaces. We extended our previous defocusing theory, valid for small defocusings, to arbitrarily large defocusings. We discovered that we can measure height fluctuations of transparent interfaces selectively, and obtain elastic properties of layered biological membranes separately. As an example, we measured separately the elastic constants associated with the two opposite surfaces of a red blood cell. The technique is very sensitive and allows us to measure the small increase of surface tension on the surface in contact with the glass-slide, as compared to the one of the free surface. Interface roughness (static and dynamic), down to nanometer amplitudes, can be measured selectively with defocusing microscopy in transparent layered materials.

12:51PM V16.00005 Terahertz spectroscopy of human skin constituents in suspension, CECIL JOSEPH, Submillimeter-Wave Technology Laboratory, University of Massachusetts Lowell, ANNA YAROLOSLAVSKY, MUNIR AL-ARASHI, Harvard Medical School, Massachusetts General Hospital, ANDREW GATESMAN, THOMAS GOYETTE, ROBERT GILES, Submillimeter-Wave Technology Laboratory, University of Massachusetts Lowell — Continuous wave terahertz imaging has the potential to offer a non-invasive medical imaging modality for detecting different types of human cancers. The aim of this study was to identify frequencies of interest for continuous wave terahertz imaging of skin cancer. The absorption characteristics of water, collagen, and elastin were studied in the range between 20 and 100cm⁻¹. In addition, we have recorded and analyzed the terahertz absorption spectra of several substances that are present in human skin (i.e. tryptophan, tyrosine, melanin, urocanic acid, keratin) and their water suspensions with the goal of using them as biomarkers for skin cancer detection.

1:03PM V16.00006 Advances in Medical X-Ray Imaging, ROBERT GOULD, University of California San Francisco — No abstract available.
1:39PM V16.00007 Inverse Participation Ratio (IPR) Analysis of Transmission Electron Microscopy (TEM) Images: Quantification of Optical Disorder Strength Due to Nanoscale Refractive Index Fluctuations of Tissues/Cells

1:51PM V16.00008 Imaging Stem Cell Aggregation Using Digital Holographic Microscopy

2:03PM V16.00009 Magnetomotive Optical Coherence Elastography for Measuring Biomechanical Properties of Tissue using Magnetic Nanoparticles

Thursday, March 13, 2008 11:15AM - 2:15PM
Session V17 GSNP DBP: Focus Session: Nonequilibrium Thermodynamics of Small Systems
Morial Convention Center 209

11:15AM V17.00001 Beyond the second law. , CHRISTIAN VAN DEN BROECK, Hasselt University — According to the second law, the work needed to bring a system from one state to another one, when in contact with a heat bath, is at least equal to the difference in free energies of these states. By a refinement of the work theorem, we derive an exact microscopic expression for the extra dissipation. It is expressed in terms of the relative entropy of the phase space density. Furthermore, lower bounds for the extra dissipation are obtained when only limited information is available. The result is illustrated on various Hamiltonian and stochastic models. The connection to the thermodynamics of computation is briefly discussed. Ref R. Kawai, JMR. Parrondo and C. Van den Broeck, Phys Rev Lett 98, 080602 (2007)

11:51AM V17.00002 Dynamics of Microtubule Growth and Catastrophe1 — SIDNEY REDNER, Boston University, TIBOR ANTAL, Harvard University, PAUL KRAPIVSKY, Boston University, MITCH MAILMAN, BULBUL CHAKRABORTY, Brandeis University — We investigate a simple dynamical model of a microtubule that evolves by attachment of guanosine triphosphate (GTP) tubulin to its end, irreversible conversion of GTP to guanosine diphosphate (GDP) tubulin by hydrolysis, and detachment of GDP at the end of a microtubule. As a function of rates of these processes, the microtubule can grow steadily or its length can fluctuate wildly. In the regime where detachment can be neglected, we find exact expressions for the tubulin and GDP concentrations. The extension of the microtubule is a random walk where the increment is a step-wise. We extract the diffusion constant and the natural frequencies of oscillation (30-200 Hz) from the time-resolved displacement traces. A microindentation apparatus was used to measure the Young’s moduli of the samples for validation and calibration with the MMOCE measurements. This novel real-time non-invasive technique affords the potential for in vivo studies.

12:03PM V17.00003 Work fluctuations in modulated systems: what is and what is not universal in the steady state , MARK DYKMAN, Michigan State University — We study work fluctuations in periodically modulated nonlinear systems. Such systems often have coexisting stable periodic states. Furthermore, lower bounds for the extra dissipation are obtained when only limited information is available. The result is illustrated on various Hamiltonian and stochastic models. The connection to the thermodynamics of computation is briefly discussed. Ref R. Kawai, JMR. Parrondo and C. Van den Broeck, Phys Rev Lett 98, 080602 (2007)

12:15PM V17.00004 Recognizing the role of microscopic reversibility in stochastic systems with optical trapping experiments as an example , ROSS BRODY, University of Maine — With optical tweezer experiments it is possible to confine a particle and observe its Brownian motion in a region of known potential. Recognizing that microscopic reversibility can lead to interesting relationships involving the particle’s motion, for example, the ratio of the conditional probability of making a transition between two points with its spatial reverse is equal to the difference between Boltzmann factors (e−ΔU/kBT), or that the time to make an up-down transition is identical to the time to make a down-up transition. With these relationships in mind, and the Onsager-Machlup action description of a path, we consider a particle in an optical tweezer of varying strength and investigate relationships involving the conditional probabilities, the actions associated with specific paths, and the external work done by varying the strength of the trap.
12:27PM V17.00005 What Do We Measure With Single-Molecule Force Spectroscopy? , CHING-HWA KIANG, NOLAN HARRIS, ERIC BOTELLO, WEI-HUNG CHEN, Rice University — Single-molecule force spectroscopy is a powerful technique for studying detailed intra- and inter-molecular interactions by manipulating single biomolecules at the nanometer scale. Force is measured while one pulls on the molecules. However, relating the measured information to equilibrium thermodynamic properties is challenging. Jarzynski’s equality allows one to reconstruct the free energy surface as a function of molecular end-to-end distance. Using protein folding as an example, we studied the parameters that influence the unfolding process, such as pulling velocity, temperature, and chemical denaturant concentration, in the solution, to demonstrate that valuable equilibrium thermodynamic information can be extracted from this technique. 1. N. C. Harris, V. Song, and C.-H. Kiang, Phys. Rev. Lett., 99 068101 (2007). 2. “Pulling Strings: Stretching Proteins Can Reveal How They Fold,” Science News, 172 22 (2007).

12:39PM V17.00006 Holographic microrheology of biofilms, FOOK CHIONG CHEONG, SIMONE DUARTE, DAVID GRIER, New York University — We present microrheological measurements of polymeric matrices, including the extra-cellular polysaccharide gel synthesized by the dental pathogen S. mutans. As part of this study, we introduce the use of precision three-dimensional particle tracking based on video holographic microscopy. This technique offers nanometer-scale resolution at video rates, thereby providing detailed information on the gels’ complex viscoelastic moduli, including insights into their heterogeneity. The particular application to dental biofilms complements previous studies based on macroscopic rheology, and demonstrates the utility of holographic microrheology for soft-matter physics and biomedical research.

12:51PM V17.00007 Fluctuation relations in a micromechanical oscillator driven far from thermal equilibrium , COREY STAMBAUGH, HÔ BUN CHAN, University of Florida — We explore fluctuation relations in a micromechanical torsional oscillator. In the linear regime when the modulation is weak, we verify that the ratio of the work variance to the mean work is independent of the driving frequency, consistent with standard fluctuation relations for a steady state system near thermal equilibrium. We then apply a strong drive to force the system into nonlinearity. Here the system displays bistability and the relationship between the work and variance is expected to deviate from the linear regime. For a bistable system the total variance has two distinct contributing components. The first results from small fluctuations about a stable state. The work variance is expected to diverge as the system approaches the bifurcation point where the state diagram changes. The other part of the variance results from the system switching between coexisting states. This part of the variance is expected to show a sharp peak near the kinetic phase transition when the populations of the two states are comparable. We compared our experimental results to theoretical predictions that distinguish nonlinear oscillators from equilibrium systems.

1:03PM V17.00008 Effect of charge distribution on the translocation of an inhomogeneously charged polymer through a nanopore , ARUNA MOHAN, ANATOLY KOLOMEISKY, MATTEO PASQUALI, Rice University — We investigate the voltage-driven translocation of an inhomogeneously charged polymer through a nanopore by utilizing discrete and continuous stochastic models. As a simplified illustration of the effect of charge distribution on translocation, we consider the translocation of a polymer with a single charged site in the presence and absence of interactions between the charge and the pore. We find that the position of the charge that minimizes the translocation time in the absence of pore-polymer interactions is determined by the entropic cost of translocation, with the optimum charge position being at the midpoint of the chain for a rodlike polymer and close to the leading chain end for an ideal chain. The presence of attractive or repulsive porecharge interactions yields a shift in the optimum charge position towards the trailing end and the leading end of the chain, respectively. Moreover, our results show that strong attractive or repulsive interactions between the charge and the pore lengthen the translocation time relative to translocation through an inert pore. We generalize our results to accommodate the presence of multiple charged sites on the polymer. Our results provide insight into the effect of charge inhomogeneity on protein translocation through biological membranes.

1:15PM V17.00009 Heat Transport in spin chains, JINSHAN WU, MONA BERCIU, UBC — The Projection operator technique, usually used to study the relaxation toward thermal equilibrium, is extended to investigate non-equilibrium but stationary processes. Particularly, in this work we apply it to study heat transport in short spin chains with Heisenberg, anisotropic Heisenberg and XY couplings plus a large magnetic field. One long-standing question is under what circumstance the relation between heat and energy is expected to deviate from the linear regime.

1:27PM V17.00010 Athermal dynamics of strongly coupled stochastic three-state oscillators, LEV TSIMRING, UCSD, BASTIEN FERNANDEZ, University of Marseille — We study the collective behavior of a globally coupled ensemble of N cyclic stochastic three-state systems with rates of transition from state i − 1 to state i proportional to the number of systems already in state i. While the mean field theory predicts only decaying oscillations in this system, direct numerical simulations indicate that the mean field exhibits stochastic oscillations even in the large N limit. We characterize the regularity of oscillations by the coherence parameter which has a well-defined maximum at the coupling constant of order 1. In contrast, the order parameter characterizing the level of synchrony among oscillators, increases monotonically with the coupling strength. We derive the exact solution of the full master equation for the stationary probability distribution and find the analytical expression for the order parameter.

1:39PM V17.00011 Entropy-driven hysteresis in a model of DNA overstretching, STEPHEN WHITE-LAM, University of Warwick, SANDER PRONK, PHILLIP GEISSLER, UC Berkeley — When pulled along its axis, double-stranded DNA elongates abruptly at a force of about 65 pN. Two physical pictures have been developed to describe this overstretched state. The first proposes that strong forces induce a phase transition to a molten state consisting of unhybridized single strands. The second picture instead introduces an elongated hybridized phase, called S-DNA, structurally and thermodynamically distinct from standard B-DNA. Little thermodynamic evidence exists to discriminate directly between these competing pictures. Here we show that within a microscopic model of DNA we can distinguish between the dynamics associated with each. In experiment, considerable hysteresis in a cycle of stretching and shortening develops as temperature is increased. Since there are few possible causes of hysteresis in a system whose extent is appreciable in only one dimension, such behavior offers a discriminating test of the two pictures of overstretched. Most experiments are performed upon nicked DNA, permitting the detachment (‘unpeeling’) of strands. We show that the long-wavelength motion accompanying strand separation generates hysteresis, the character of which agrees with experiment only if we assume the existence of S-DNA.

1:51PM V17.00012 Replica and extreme-value analysis of the Jarzynski free-energy estimator, MATTEO PALASSINI, FELIX RITORT, Department of Fundamental Physics, University of Barcelona — We analyze the Jarzynski estimator of free-energy differences from nonequilibrium work measurements. By a simple mapping onto Derrida’s Random Energy Model, we obtain a scaling limit for the expectation of the bias of the estimator. We then derive analytical approximations in three different regimes of the scaling parameter x = log(N)/W, where N is the number of measurements and W the mean dissipated work. Our approach is valid for a generic distribution of the dissipated work, and is based on a replica symmetry breaking scheme for x ∝ 1, the asymptotic theory of extreme value statistics for x ≳ 1, and a direct approach for x near one. The combination of the three analytic approximations describes well Monte Carlo data for the expectation value of the estimator, for a wide range of values of N, from N=1 to large N, and for different work distributions. Based on these results, we introduce improved free-energy estimators and discuss the application to the analysis of experimental data.
Ib-PS field effect transistor at various temperatures. We show that the current voltage characteristic at different temperatures follow SCLC type conduction. In this talk we present electronic transport characteristics of poly(3-hexylthiophene) block poly(styrene) copolymer (rr-P3HT). To properly utilize these new types of materials it is necessary to understand the relationship between their molecular structure and electronic transport properties of rr-P3HT. Previous studies have shown that symmetric PSS-PMB block copolymers in the presence of humid air (relative humidity > 50%) are excellent proton conductors at temperatures as high as 90°C. Current work is focused on water uptake and conductivity measurements on asymmetric PSS-PMB block copolymers with PSS as the minor component.

1 The primary author of this paper is Moon Jeong Park. This work was supported by the Office of Basic Energy Sciences of the USDOE.

12:03PM V18.00003 Temperature dependent charge transport properties of poly(3-hexylthiophene) block poly(styrene) copolymer field-effect transistor, Firoze Haque, Paul Stokes, Lei Zhai, Saiful I. Khondaker, Nanoscience Technology Center, Departments of Physics and Chemistry, University of Central Florida Team — Regioregular poly-3-hexylthiophene (r-P3HT) is considered to be one of the most promising and well studied organic semiconductors. Recently attention has been focused on developing di-block copolymers of rr-P3HT by attaching non-conjugated blocks which allows one to tune the electrical properties of rr-P3HT. To properly utilize these new types of materials it is necessary to understand the relationship between their molecular structure and electronic transport properties. In this talk we present electronic transport characteristics of poly(3-hexylthiophene) block poly(styrene) copolymer (r-P3HT-b-PS) field effect transistor at various temperatures. We show that the current voltage characteristic at different temperature follow SCLC type conduction mechanism with $I \propto V^n$, where $n$ varies from 1.5 to 2.2. We also show that the room temperature hole mobility is $\sim 3.5 \times 10^{-5}$ cm$^2$/Vs, and that the mobility decreases with decreasing temperature. The temperature dependent mobility follow activated hopping process. The space charge limited current along with the low mobility of the devices indicates that the charge transport is limited by the insulating poly styrene segment of the di-block polymer.

1 The authors thank Kraton LLC and Dexcel for copolymer samples. Major support for these studies from the National Science Foundation Materials Research Science & Engineering Center (DMR 0213883 - USM) and NSF MRSEC DMR 0213985 (UA) is acknowledged.
12:27PM V18.00005 The Lyotropic Phase Behavior of Diblock Copolymers Swollen with Ionic Liquids. PETER SIMONE, University of Minnesota Department of Chemistry, TIMOTHY LODGE, University of Minnesota Department of Chemistry and Department of Chemical Engineering and Materials Science — The lyotropic phase behavior of poly(1,2-butadiene-co-ethylenoxide) (PB-PEO) has been studied upon addition of two ionic liquids, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMI][TFSI]) and 1-butyl-3-methylimidazolium hexafluorophosphate ([BMI][PF6]). The copolymer/ionic liquid samples ranged from dilute to concentrated, and were characterized via small angle X-ray scattering (SAXS) and cryogenic transmission electron microscopy (cryo-TEM). At moderate to high concentrations, SAXS patterns corresponding to the classical copolymer microstructures of body-centered cubic lattices of spheres, hexagonally packed cylinders, and lamellae were observed. Additionally, at several concentrations, coexisting microstructures and what is thought to be a disordered network microstructure were observed. At low concentration, the morphology of the block copolymer micelles (i.e., spheres, cylinders, and vesicles) was used as a qualitative gauge of the ionic liquid solvent quality, and it was concluded that for PB-PEO, [BMI][PF6] behaves as a more selective solvent than [EMI][TFSI].

1 Supported by the National Science Foundation award DMR-0406656

12:39PM V18.00006 Structure and Thermodynamics of Block Copolymers Doped with Ionic Liquids. J.M. VIRGILI, N.P. BALSARA, R.A. SEGALMAN, University of California, Berkeley — Incorporation of ionic liquids into block copolymers is of interest for applications such as high temperature fuel cell membranes and polymer processing. These applications take advantage of ionic liquids' attractive physicochemical properties, such as low vapor pressure and high thermal stability. We investigate the structure and thermodynamics of poly(styrene-b-2-vinylpyridine) (PS-PVP) block copolymers doped with an ionic liquid consisting of imidazole and bis(trifluoromethanesulfonyl)amide (HFTSI). Using small angle X-ray scattering (SAXS), we demonstrate that increased ionic liquid doping leads to swelling of lamellar nanodomains in a symmetric PS-PVP block copolymer. At high ionic liquid loadings, we observe break up of the lamellar domains into hexagonally perforated lamellae. We characterize the effect of ionic liquid loading on the order-disorder transition (ODT) temperature of PS-PVP. We observe depression of the PS-PVP ODT temperature with increasing loading of the ionic liquid.

12:51PM V18.00007 Controlling the morphology of liquid crystalline block copolymers: interfacial and liquid crystal content effects. ERIC VERPOELEN, TEJIA ZHANG, PAULA HAMMOND, MIT — By systematically controlling the covalent attachment of side chain liquid crystals to a block copolymer backbone, the morphology of both the liquid crystalline (LC) mesophase and the phase segregated BCP microstructures can be precisely manipulated. A wide range of morphologies can be achieved from a single block copolymer backbone during a one step LC attachment reaction. The anchoring of the smectic LC mesophase to the inter-molecular dividing surface (IMDS) is a key driving force in determining the morphologies for both the bulk and in thin films. In thin films the orientation of the morphology is determined by the minimization of the surface energy with the substrate and air interfaces and the anchoring of the LC mesophase to the substrate. These competing effects can be utilized to manipulate the orientation of as-cast and thermally annealed thin films. Additionally, by controlling the LC content, the mechanical properties of this system can be tailored over a several orders of magnitude. The tune-ability demonstrated in this system will allow for custom design and tailoring of material properties for specific applications such as electromechanical and mechno- optical devices.

1:03PM V18.00008 Self-assembly of side chain liquid crystalline block copolymers. MANAS SHAH, VICTOR PYRAMITSYN, VENKAT GANESAN, University of Texas at Austin — We present a new model based on self-consistent field theory (SCFT) approach to characterize the self assembly behavior in side-chain liquid crystalline block copolymers. Our model considers a micromechanical representation of flexible coil-coil diblock copolymers, with rod-like units grafted to one of the blocks. We present results which elucidate self-assembly arising from the interplay between block copolymer microphase separation and the orientational ordering of the rod segments. Our numerical results are in very good agreement with reported experimental observations. Many of the traditional flexible diblock copolymer microphases are also predicted to occur for side chain liquid crystalline copolymers, with smectic ordering accompanying within the microphases. The equilibrium phase morphologies are observed to depend on the molecular weight of the copolymer, the length of the rod units, the relative volume fractions of each block, and the energetic and orientational interactions between different components. Moreover, for the parameters considered in this article, microphase separation was observed to be a requisite for developing orientational ordering between mesogenic units.

1:15PM V18.00009 Structural Formation Process of Microphase Separated Films with Liquid Crystalline Phase Transition. MOTONORI KOMURA, TOMOKAZU IYODA, Tokyo Institute of Technology — Ordered nanostructures arising from the microphase separation of block copolymers have driven one to fabricate nanofunctional materials as fundamental technology of the coming electronic and photonic materials. Thin films of a series of newly designed amphiphilic block copolymer consisting of hydrophilic polyethylene oxide (PEO) and hydrophobic polymethacrylate with azobenzene-mesogen in side-chain (PMA(Az)) show highly ordered microphase separation with PEO cylinders perpendicularly oriented to the film surface. In the present report, we investigated a structural formation process of the microphase separated films by temperature controlled atomic force microscopy (AFM) and grazing incidence small angle X-ray scattering (GISAXS). These measurements revealed that homeotropic alignments of Az liquid crystalline layers predominated the cylinder orientation, which corresponded to a <110> direction of body centered cubic structure under annealing condition, in disagreement with cylinder orientation of order-order transition of traditional block copolymers.

1:27PM V18.00010 Rod-to-Coil Transition in Polyoligo(9,9-dihexylfluorene-2,7-diyl) diblock copolymers. RAFFAELE MEZZENGA, LAURENT RUBATAT, Fribourg University, Physics Department, Switzerland, XIANGXING KONG, SAMSON JENEKHE, University of Washington, Seattle, USA, JANNE RUOKOLAINEN, Helsinki University of Technology, Finland, MOHAMAD HOJEIJ, EPFL, Switzerland — Self-assembly in the bulk of a series of hybrid triblock copolymers formed by a poly(9,9-dihexylfluorene-2,7-diyl) internal block and two poly(9,9-dihexylfluorene-2,7-diyl) end blocks has been studied. Since the α-helical secondary structure of the PBLG block may be either maintained or suppressed depending on the solvent casting history, the PBLG-PFH-PBLG copolymers exhibit two different conformations: a rod-rod or coil-rod configuration, respectively. To provide insight on the influence of molecular architecture on self-aggregation of these systems, three copolymers with different block ratio were investigated in both conformations using small- and wide-angle scattering techniques and transmission electron microscopy. Time-resolved photoluminescence measurements were performed on the same samples to explore the effect of morphology on photophysical properties. The observed photoluminescence spectra and dominant excited lifetimes of the poly(9,9-dihexylfluorene-2,7-diyl) block were found to differ markedly in rod-rod and coil-rod configurations and were correlated to the morphology of the self-assembled triblock copolymers.

1:39PM V18.00011 The effect of chain stiffness on the morphology of diblock copolymers. G. LEUTY, J. BEDARD, MESFIN TSIGE, Southern Illinois University — One of the most interesting and challenging problems in the science of materials concerns the structure and dynamics of the morphology of block copolymers. These materials generally consist of two or more homopolymer chains or blocks that are covalently bonded to each other to form a single polymer chain. Variation in the stiffness of the different block segments can directly affect the morphology of the system and may thus result in a very rich phase behavior. In the present study, the microphase separation of symmetric diblock copolymers with variable block stiffness and chain length is studied using coarse-grained molecular dynamics simulations. In the lamellar phase, the equilibrium lamellar spacing and orientation of the block segments in the system are found to depend on the relative stiffness between the two block segments. As the chain length of the block segments increases, the morphology changes from the expected lamellar appearance to a cylindrical one.
1:51PM V18.00012 Self-assembled OLEDs from rod-coil block copolymers. Y. TAO, R.A. SEGALMAN, University of California Berkeley and Lawrence Berkeley National Lab — High efficient OLEDs tend to be made of many stacked layers including layers for hole transport, emission, and electron transport, which are produced via a very tedious sequence of high vacuum steps. Since conjugated rod-coil block copolymers form layer structures due to rod-coil repulsions and rod-rod interactions, they are an alternate route towards multi-layer devices which can be solution processed in one single step. A functional conjugated rod-coil block copolymer, poly(alkoxyphenylene vinylene-b-oxadiazole (PPV-b-OX)), incorporates a hole transporting/emissive rod and an electron transporting coil. Grazing Incidence X-ray scattering is used to demonstrate the layered structure of the resulting self-assembled block copolymer film relative to the substrate (electrode). A multi-layer thin film self-assembled from PPV-b-OX shows significant improvement in luminescence and efficiency over pure PPV and PPV/OX blend devices. The correlation between details of thin film structure including lamellar spacing, orientation, and number of layers and device performance will also be discussed.

2:03PM V18.00013 Self-assembly of linear rod-coil block copolymers. LI-JIA AN, JI-ZHONG CHEN, ZHAO-YAN SUN, CHENG-XIANG ZHANG, Changchun Institute of Applied Chemistry, CAS — Rod-coil block copolymer systems have attracted a great deal of attention due to their rich phase behavior. The spontaneous ordering of coil-rod block copolymers is due to the mutual repulsion of the dissimilar blocks and the packing constraints imposed by the connectivity of each block, while the stiff rigidity of the rod segment imparts orientation organization. However, few reports investigate rod-coil block copolymers in three-dimension space. In this work, the self-assembly of linear rod-coil block copolymers is studied by applying self-consistent-field lattice techniques in three-dimension space. The stiffness influences on the self-assembly and the possible orientations of the rods in different structures are focused on for rod-coil diblock copolymers; the interfacial grafting density of the separating rod and coil segments is found exerting important influences on the phase behavior of symmetric coil-rod-coil triblock copolymers; the influences of the intramolecular interactions between the two rods of the symmetric rod-coil-rod triblock copolymer chain on the self-assembly are studied.

1 This work is supported by the NSFC Programs (20490220, 20674086 and 50621302), and subsidized by the Special Funds for National Basic Research Program of China (2005CB623800).


11:15AM V19.00001 Mechanochemistry of Molecular Motors. ZEV BRYANT, Stanford University Schools of Medicine and Engineering — Molecular motors lie at the heart of biological processes from DNA replication to vesicle transport. We seek to understand the physical mechanisms by which these nanoscale machines convert chemical energy into mechanical work. I will overview our ongoing use of single molecule tracking and manipulation techniques to observe and perturb substeps in the mechanochemical cycles of individual motors, before concentrating on our recent efforts to dissect the structural basis of a “reverse gear” in myosin VI. The basic actomyosin motor has been embellished, altered, and re-used many times through the evolution of diverse members of the myosin superfamily. Class VI myosins are highly specialized (-) end directed motors involved in a growing list of functions in animal cells, including endocytosis, cell migration, and maintenance of stereociliar membrane tension. How does myosin VI achieve reverse directionality, despite sharing extensive sequence and structural conservation with (+) end directed myosins? We generated a series of truncated myosin VI constructs and characterized the size and direction of the power stroke for each construct using dual-labeled gliding filament assays and optical trapping. Motors truncated near the end of the converter domain generate (+) end directed motion, whereas longer constructs move toward the (-) end, confirming the importance of a class-specific insert that redirects the lever arm. Our quantitative results suggest a surprising model in which the lever arm rotates ~180° during the power stroke. We are currently studying the behavior of engineered myosin VI constructs with artificial lever arms, in order to further challenge and refine our power stroke model.

11:51AM V19.00002 Rare returns on lost effort! Dynamic refolding (after unfolding) of protein domains. EVAN EVANS, Boston University — Dynamic force loading is an established technique for probing the forward kinetics in unfolding of single protein domains. Examined over several orders of magnitude in force rate, the unfolding forces often exhibit a linear dependence on the logarithm of loading rate, revealing the dynamic truncation of a precipitously activation barrier. The slope and force-rate intercept of the linear response characterize the critical molecular length gained in the barrier transition and the force-free rate of barrier passage. On the other hand, if reversed and probed with negative force rates, refolding of a stretched polypeptide chain has been found to yield a linear relation between the squares of the refolding forces and the logarithms of (reverse) force rates. Revealing here the dynamic elevation of a deep harmonic well that confines the unfolded states, the slope and force-rate intercept of the linear response also characterize the effective spring constant of the harmonic well and the unstretched refolding rate. Representing a dynamical corollary to predictions of fluctuation theorems for small systems, the most-frequent amount of mechanical work recovered (from the thermal environment) in refolding increases with each decade reduction in the force-unloading rate and approaches the limit set by near-equilibrium transitions over a logarithmic span related to the free energy of transition.

1 Acknowledgement: supported by USDA NIH Grants HL31579 and HL65333.

12:27PM V19.00003 Generalization of distance to higher dimensional objects, and its application to protein folding. STEVEN PLOTKIN, University of British Columbia — After a brief biophysical introduction to motivate the problem, I will show how the notion of calculation of distance between two objects can be generalized to the case where the objects are no longer points, but are one-dimensional. Additional concepts such as nonextensibility, curvature constraints, and noncrossing become central to the notion of distance. I will give some analytical and numerical results for specific examples, and I will discuss applications to biopolymers and protein folding.

1 Support from NSERC and the A.P. Sloan Foundation are gratefully acknowledged.

1:03PM V19.00004 Getting into shape: the physics of bacterial morphology. KERWYN HUANG, Princeton University — Bacterial cells come in a wide variety of shapes and sizes, with the peptidoglycan cell wall as the primary stress-bearing structure that dictates cell shape. In recent years, cell shape has been shown to play a critical role in regulating many important biological functions including attachment, dispersal, motility, polar differentiation, predation, and cellular differentiation. Though many molecular details of the composition and assembly of the cell wall components are known, how the peptidoglycan network organizes to give the cell shape during normal growth, and how it reorganizes in response to damage or environmental forces have been relatively unexplored. We introduce a quantitative mechanical model of the bacterial cell wall that predicts the response of cell shape to peptidoglycan damage in the rod-shaped Gram-negative bacterium Escherichia coli. To test these predictions, we use time-lapse imaging experiments to show that damage often manifests as a bulge on the sidewall, coupled to large-scale bending of the cylindrical cell wall around the bulge. The direction of the symmetric rod-coil-rod triblock copolymer chain on the self-assembly are studied.

This work was funded by NIH grants 5K25 GM075000 and R01 GM073186.
The ability to sense changes in the environment allows bacteria to respond by altering their phenotype, or behavior, to adapt to new conditions. Alternatively, bacteria have the ability to spontaneously change their phenotype, without sensing. Such behavior is known as stochastic switching. By simply observing dividing bacteria, is it possible to tell whether the cells are sensing their environment? This talk presents a theory that can decouple the action of sensing from the action of natural selection using single-cell observation of bacteria.

Thursday, March 13, 2008 11:15AM - 2:03PM —
Session V20 DCMP: Phase Transitions: Structural, Electronic, and Magnetic Morial Convention Center 212

11:15AM V20.00001 Inequivalent Down Atom (3x3) structure in Sn/Ge(111) , R. CORTES, Dpto. Fisica Materiales, Univ. Complutense, Spain, A. TEJEDA, MPQ, CNRS, France, J. LOBO-CHECA, Dpt. of Physics, Univ. of Basel, Switzerland, C. DIDIOIT, B. KIERREN, D. MALTERRE, LPM, Univ. Henri Poincare, France, E.G. MICHEL, Dpto. Fisica Mat. Condensada, Univ. Autonoma de Madrid, Spain, A. MASCARAO, Dpto. Fisica Materiales, Univ. Complutense, Spain — The (3x3) phase of Sn/Ge(111) is formed by three Sn atoms in the unit cell, one of them at a higher level than the other two (1-up, 2-down model). Although this model is mostly accepted, it is still controversial because of apparently contradicting experimental results related to the Sn 4d core level line shape. This work reports on high-resolution photoemission spectroscopy (HR-PES) and scanning tunnelling microscopy (STM) experiments on Sn/Ge(111)-(3x3). Our PES data resolve three main components in the Sn 4d core level [1] instead of two found before [2], which are assigned to the three Sn atoms in the unit cell. This indicates that the two down atoms are at slightly different heights, forming an inequivalent-down-atoms (IDA)-(3x3) structure, also confirmed by STM images. These results conclusively solve the long-standing controversy [2] on the interpretation of the Sn 4d core level line shape, and support a model fully consistent with an initial state picture. [1] A. Tejeda et al. Phys. Rev. Lett. In press [2] R.I.G. Uhrberg et al., Phys. Rev. Lett. 85, 1036 (2000) and references there in.

11:27AM V20.00002 Formation of $\sqrt{3}\times\sqrt{3}$ structure by depositing Si on Si(111)-(5x2)/Au1 . F.-K. MEN, A.-L. CHIN, C.-F. JAN, J.-L. GUO, Department of Physics, National Chung Cheng University, Chia-Yi, Taiwan, R.O.C. — By depositing Au on a Si(111) surface at an elevated temperature, 5x2, $\sqrt{3}\times\sqrt{3}$, and 6x6 reconstructions emerge successively as the Au coverage increases. Though great efforts have been made to identify atomic models for each reconstruction, satisfactory result is still lacking. By depositing Si on a 5x2 surface, we have identified the formation of the $\sqrt{3}\times\sqrt{3}$ structure even there was no additional Au being deposited. This observation leads us to speculate (i) the $\sqrt{3}\times\sqrt{3}$ structure has a higher Si density than that of the 5x2 structure, and (ii) the Au density in a single-domain $\sqrt{3}\times\sqrt{3}$ structure, i.e., no domain walls, is roughly equal to that in the 5x2 structure.

11:39AM V20.00003 Temperature-induced Self-pinning and Nano-layering of AuSi Eutectic Droplets , NICOLA FERRALIS, ROYA MABOUDIAN, CARLO CARRARO, University of California at Berkeley — A process for self-pinning of AuSi eutectic alloy droplets to a Si substrate, induced by a controlled temperature annealing in ultra-high vacuum, is presented. Surface pinning of AuSi 3D droplets to the Si substrate is found to be a consequence of the readjustment in the chemical composition of the droplets upon annealing, as required to maintain thermodynamic equilibrium at the solid-liquid interface. Structural and morphological changes leading to the pinning of the droplets to the substrate are analyzed using atomic force microscopy, scanning and transmission electron microscopy. Raman spectroscopy measurements performed on the droplets reveal phase separation upon cooling of the droplets, leading to the formation of amorphous Si-rich channels within the core, and the formation of crystalline Si nanoshells on the outside. The mechanism leading to the pinning and surface layering provide new insight into the role of alloying during growth of silicon nanowires and may be relevant to the engineering of nano-scale Si cavities. We shall also present measurements of the diffusion of Au drops on Si(111) obtained by low-energy electron microscopy.

11:51AM V20.00004 Adsorbate-Induced Faceting of Ir and Re Surfaces , PAYAM KAGHAZCHI, TIMO JACOB, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, 14195 Berlin, Germany, WENHUA CHEN, HAO WANG, THEODORE MADEY, Rutgers University, NJ 08854, USA — Since high-index clean metal surfaces typically have lower surface atom densities and higher surface free energies compared to the close-packed surfaces of the same metal they can be used as the basis for surface reconstruction and facet formation studies. In this context experimentally we found recently that on Ir(210) and Re(111) surfaces strongly interacting adsorbates are able to induce the formation of well defined nanostructures after annealing the system at elevated temperatures. Using density functional theory calculations with the PBE functional and \textit{ab initio} atomistic thermodynamics we studied the adsorption of oxygen and nitrogen on the different surface orientations, which are involved in the nanostructures on Ir(210) and Re(111). Constructing the corresponding (p, T)-surface phase diagrams, we find that at experimental pressure conditions ($P_{O_2} = 5 \times 10^{-10}$ atm) above 1100K for Ir and above 1200K for Re the planar surfaces are stable, while lowering the temperature stabilizes the nanofacets found experimentally. While on Ir(210) most nanoscale pyramids consist of smooth and unreconstructed planes, some (110) facets show a stepped double-missing row superstructure, which is only stable on the faceted surface and at higher temperatures.

12:03PM V20.00005 Oxygen-induced nanoscale pyramidal faceting of Rh(210) surface , GOVIND ., W. CHEN, H. WANG, THEODORE E. MADEY, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854, USA — The adsorption of oxygen and nanometer-scale faceting induced by oxygen have been studied on atomically-rough fcc Rh(210) using LEED and AES. The Rh(210) surface remains planar at room temperature after being exposed to oxygen. Upon annealing at temperatures above 600K, Rh(210) covered by \textasciitilde{}1ML of oxygen undergoes reconstruction to form 3-sided nanoscale pyramids characterized by two (731) facets and a (2x1)-reconstructed (110) facet. The surface remains faceted for T up to 850K. Oxygen can be completely removed from the faceted surface via CO oxidation at 400K or reaction with H$_2$ at room temperature, while preserving the faceted structure. The clean faceted surface remains stable below 600K and irreversibly relaxes to the planar surface at higher temperatures. The clean faceted Rh(210) surface is a potential substrate to study surface reactions whose rates are sensitive to atomic structure and/or nanoscale (facet) size. The results are compared with measurements of oxygen-induced faceting of Ir(210). Work supported by DOE, Office of basic Energy Science
12:15PM V20.00006 Order-disorder phase transition of the Cu(001) surface under equilibrium oxygen pressure. H. IDDAR, D.D. FONG, MSD, Argonne National Laboratory, IL 60439, P. ZAPOL, CSED & MSD, Argonne National Laboratory, IL 60439, P.H. FUOSS, MSD, Argonne National Laboratory, IL 60439, L.A. CURTISS, CSED & MSD, Argonne National Laboratory, IL 60439, G.-W. ZHOU, J.A. EASTMAN, MSD, Argonne National Laboratory, IL 60439 — Understanding atomic processes involved in catalyzed reactions is of great importance and can be achieved by studies of adsorbate-induced surface structures. Copper catalysts are heavily used in methanol and formaldehyde synthesis, two reactions in which oxygen adsorption is an important intermediate step. To better understand catalytic reactions, it is imperative to both identify and characterize the atomic structure of all phases present on metal surfaces at elevated temperatures and pressures relevant to working catalysts. We will report on our discovery of a new high-temperature oxygen-induced surface phase on Cu (001) using a combination of in situ synchrotron x-ray scattering and first-principles theory. This high-temperature phase is characterized by 1/4 ML of randomly-distributed vacancies in the topmost Cu layer with a c(2x2)-O adlayer. Below 473 K a reversible transition to a $\sqrt{2} \times \sqrt{2}$ R45° missing row phase occurs. The results show that this entropy-driven phase transition occurs through the diffusion of Cu vacancies underneath the oxygen superstructure. This work is supported by DOE BES under Contract # DE-AC02-06CH11357.

12:27PM V20.00007 Ab initio phase diagram of oxygen adsorption on W(110)1. MARKUS STÖHR, University of Vienna, Department of Physical Chemistry, STEFFAN MÜLLER, University of Erlangen-Nuremberg, Chair of Solid State Physics, RAIMUND PODLOUCKY, University of Vienna, Department of Physical Chemistry — Oxygen adsorption on the tungsten (110) surface has been studied experimentally as well as by semi-empirical theoretical approaches. Up to now, no ab initio modelling of this adsorption process has been done, for which we present a combined density functional theory (DFT) and cluster expansion (CE) study. For the CE all lateral unit cells with up to 12 atoms were considered. The (2x1) and (2x2) adsorption phases are found to be ground states which is confirmed experimentally [1]. On the basis of effective cluster interactions Monte Carlo (MC) simulations were performed in order to access finite temperature effects. Concerning the atomic structure we find excellent agreement to experimental scanning tunneling microscopy studies [2]. The temperature and coverage dependent short range order parameter is analyzed. From the results of the applied DFT, CE and MC approaches an ab initio surface phase phase diagram can be derived. [1] Wu et al., Physical Review B 39, 7595 (1989). [2] Johnson et al., Phys. Rev. Lett., 71, 1055 (1993).

1Work supported by FWF project nos. WK4 and S90.

12:39PM V20.00008 Lattice gas transition of xenon on a fullerite surface1. SILVINA GATICA, Department of Physics, Howard University, MILTON COLE, Department of Physics, Pennsylvania State University — We study a lattice-gas transition of xenon atoms on a honeycomb geometry. It is found from experiments and Monte Carlo simulations that this configuration occurs for xenon adsorbed on a substrate consisting on an array of C60 molecules on Ag(111). At very low coverage the atoms occupy strong-binding 3-fold hollow sites between C60 molecules. In this way, they form a commensurate lattice with nearest neighbor distance 0.58 nm. Using a Lennard Jones model for the Xe-Xe potential, the nearest neighbor interaction strength is $U=96.7$ K. Using the Ising model we estimate the transition critical temperature to be $T_c=30$ K. We compare with our results from Monte Carlo simulations based on more realistic interactions.

1Research supported by NSF. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

12:51PM V20.00009 Stability of the commensurate monolayer solid of xenon/graphite. L.W. BRUCH, Department of Physics, University of Wisconsin-Madison, A.D. NOVACO, Department of Physics, Lafayette College — A stability analysis based on model calculations of the grand potential finds that the transition from hexagonal incommensurate to commensurate monolayer solid of xenon/graphite is continuous with increasing pressure, in agreement with experimental observations. An atomic-scale interaction model gives an internally consistent account of the thermal expansion of the solid at the 2D sublimation curve and of the chemical potential increase for isothermal compression from monolayer condensation to the commensurate solid. An estimate is given for the corrugation energy of xenon/graphite.

1:03PM V20.00010 Molecular dynamics simulations of hexane on graphite at various coverages: the difference explicit hydrogens make1. M.W. ROTH, M.J. CONNOLLY, University of Northern Iowa, Department of Physics, PAUL A. GRAY, University of Northern Iowa, Department of Computer Science, CARLOS WEXLER, University of Missouri Columbia, Department of Physics and Astronomy — Molecular Dynamics simulations of hexane (C6H14) adlayers on graphite are carried out for coverages of 0.5 $\leq \rho \leq$ 1 monolayers. The hexanes have explicit hydrogens and the graphite is modeled as an all - atom, six - layer structure. Above $\rho \cong$ 0.9 the herringbone solid loses orientational order at $T_1=140$ K $\pm$ 3 K. At $\rho = 0.878$ the system presents vacancy patches and $T_1$ decreases to ca. 100 K. As coverage decreases further, the vacancy patches become larger and by $\rho = 0.614$ the solid is a connected network of randomly oriented domains. All cases show a weak nematic mesophase. The melting temperature is $T_2=160$ K $\pm$ 3 K and falls to ca. 145 K by $\rho = 0.614$. The dynamics and energetics observed demonstrate that the explicit-hydrogen model of hexane is substantially more realistic than the UA approximation.

1Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund (PRF43277 - B5), the University of Missouri Research Board, and the D.O.E. (DE-FG02-07ER46411).

1:15PM V20.00011 Molecular Dynamics study of tetracosane monolayers adsorbed on graphite1. L. FIRLEJ, B. KUCHTA, M.W. ROTH, University of Northern Iowa, Department of Physics, PAUL A. GRAY, University of Northern Iowa, Department of Computer Science, CARLOS WEXLER, University of Missouri Columbia, Department of Physics and Astronomy — We present the results of Molecular Dynamics (MD) simulations of tetracosane (C24H50) monolayers physisorbed on graphite. C24H50 molecules have explicit hydrogens and the graphite is represented by six graphene layers. We focus our analysis on the microscopic mechanism of melting, experimentally observed at T = 340 K. We are looking for the pre-melting transformations with emphasis on the correlation between translational disordering of molecules and their internal degrees of freedom. We analyze several order parameters and their fluctuations along the MD trajectories. We show that the all atom representation of C24H50 is much more sensitive to the model of intramolecular interactions than united atom model. Footprint reduction during melting involves a simultaneous loss of intramolecular and translational order.

1Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund (PRF43277 - B5), the University of Missouri Research Board, and the D.O.E (DE-FG02-07ER46411).
1:27PM V20.00012 Test of the universality of the scaling energy in alkanes using melting transition of layer adsorbed on graphite

B. KUCHTA, L. FIRLEJ, M.W. ROTH, University of Northern Iowa, Department of Physics, PAUL A. GRAY, University of Northern Iowa, Department of Computer Science, CARLOS WEXLER, University of Missouri Columbia, Department of Physics and Astronomy — The non-bonded terms together with the torsional energy determine the internal (conformational) degrees of freedom of simulated alkanes. Being able to predict the energy and ordering of conformations correctly is an essential quantity for bringing force field methods into the predictive regime of theoretical methods. To estimate the universality of modern force fields it is helpful to know how different components of classical fields affect the simulated properties. In the case of alkanes, the interplay between torsion potential and the scaling of 1-4 van der Waals and 1-4 charge-charge (QQ) interactions plays a crucial role. It is the purpose of this work to study universality of the scaling factor of 1-4 non-bonded interactions in alkanes. Three alkanes of length from 7 to 30Å (C₇, C₁₂, C₂₄), in an all-atom representation have been analyzed.

1:39PM V20.00013 Heisenberg Spin Systems with Long Ranged Couplings

UTE LÖW, Universität Dortmund, Institut fuer Physik, D44221 Dortmund — Static correlation functions of Heisenberg spin systems with various (non-frustrated) topologies are studied by means of Quantum-Monte Carlo techniques. In particular dimerizations and longer ranged variations of spin couplings and alternations between ferromagnetic and anti-ferromagnetic couplings are considered. The phenomenology of possible ground state phase diagrams is discussed.

1:51PM V20.00014 Hysteresis in the anomalous Hall effect of MnAs thin films

FELIX T. JAECKEL, ANDREAS STINTZ, ABDEL-RAHMAN A. EL-EMAWY, KEVIN J. MALLOY, Center for High Technology Materials, University of New Mexico, 1313 Goddard St. SE, Albuquerque, NM 87106 — We report detailed measurements of the Hall effect in MBE-grown MnAs thin films on (001)-GaAs as a function of temperature. Hysteresis of the Hall resistivity is observed for temperatures between 300 and 355 K. Non-linear behavior of the Hall resistivity persists up to 390 K. The appearance of hysteresis at low temperatures can be explained by the emergence of stable, out-of-plane domains due to the shape anisotropy of the contracting α-phase. However, the persistence of the hysteresis and the anomalous Hall effect at temperatures significantly above 318 K is not consistent with the complete transformation of the α-phase and introduces new questions about the magnetic properties of the β-phase.

Thursday, March 13, 2008 11:15AM - 2:03PM — Session V21 DPOLY: Charged and Ion-Containing Polymers I Morial Convention Center 213

11:15AM V21.00001 Nano-Patterns in Gels of Charged Chains with Self-Attracting Interactions

MONICA OLVERA DE LA CRUZ, Northwestern University, JUAN J. DE PABLO, University of Wisconsin-Madison — Gels of weakly charged chains have large swelling capabilities that depend on pH and/or salt concentration. In the presence of attractions among elastic units, such as poor-solvent conditions, stable nano-patterns are observed. These systems are ideal actuators, since they undergo large volume changes at the nanophase transition. We find that the nanophases are due to the entropy of the counterions, and are stabilized as the monomer density decreases and as the salt concentration increases by hard-core interactions and network heterogeneities. Our model is constructed with results from a non-linear Poisson Boltzmann approach in the limits when it is applicable (low ionic densities) and a grand canonical Monte Carlo method simulation with Donnan partitioning of counterions and co-ions between the gel and reservoir phases. Our theory and simulations are in close agreement with experiments.

11:27AM V21.00002 Interactions in Ion-containing Polymers Probed by ab initio Methods

WENJUAN LIU, RALPH COLBY, Materials Science and Engineering Department, The Pennsylvania State University, MICHAEL JANIK, Department of Chemical Engineering, The Pennsylvania State University, THE PENNSYLVANIA STATE UNIVERSITY TEAM — We use ab initio methods to estimate dipole moments and interaction energetics in ion-containing polymers. Our calculation quantitatively includes electrostatic interactions (using both permanent and induced dipoles) and effectively estimates solvation energetics for ions interacting with various functional groups. Interactions are reported for various small cations with common functional groups on polymers and carboxylate, sulfonate and phosphonate groups that can be present in anionic ionomers. We demonstrate how these interaction energies can be utilized to design polymer membranes with facile ion transport.

11:39AM V21.00003 Conformation transition and counterion distribution of single polyelectrolyte chains in aqueous solution

JIAN ZHAO, SHENQIN WANG, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — We adopted single fluorescence techniques to study the conformation transition of poly 2-vinylpyridine in its aqueous solution. The first-order conformation transition from extended coil to collapsed globule was observed as the pH value in the solution was raised. The critical pH value was shifted higher largely upon the addition of salt in the solution. The study shows a difference of proton concentration at the chain to that in the solution (a difference of three orders of magnitude), and the addition of salt in the solution increased the local proton concentration at the chain and therefore shift the transition point.

11:51AM V21.00004 Unifying Self-Consistent Field Theory for Weak Polyelectrolytes

KEVIN WITTE, YOU-YEON WON, Purdue University — A self-consistent field (SCF) theory for weak polyelectrolytes has been derived from a grand canonical partition function. The formalism accounts for the location and mixing of the charged and uncharged polymer species, treating the local (spatially dependent) charge fraction as a field variable with which to minimize the total free energy. This method of the derivation gives the resulting equations, especially those governing the local charge fraction, that are identical to the results obtained by Szeifer and coworkers (J. Polym. Sci. B Polym. Phys., 2006) who built upon the mean-field “annealed” free energy expression proposed by Raphael and Joanny (Europhys. Lett., 1990). However, we show that these results are further identical to the “two-state” model of Borukhov, Andelman and Orland (Eur. Phys. J. B, 1998), namely, the potential field due to the polymer charges with which the chains interact and the local charge fraction are shown to be exactly equal. This annealed model is derived by averaging the partition function with regard to the monomer charges. The charged and uncharged states are weighted by their probabilities which is, in our notation, the bulk charge fraction and one minus the bulk charge fraction, respectively. The utility of this theory is demonstrated by comparing its predictions against various experimental results from bulk potentiometric measurements and also from poly electrolyte brush compression studies.

1 Project supported by The National Natural Science Foundation of China (NSFC)
12:03PM V21.00005 Composition and Structure Changes of the Ionic Aggregates with Acid Content and Neutralization Level in Poly (styrene-co-methacrylic acid) Ionomers. WENQIN WANG, TSUNG-TA CHAN, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6272. ANDREW PERKOWSKI, SHULAMITH SCHLICK, Department of Chemistry and Biochemistry, University of Detroit Mercy, Detroit, Michigan 48221, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104 — The morphology of poly(styrene-co-methacrylic acid) (SMAA) copolymers neutralized with copper(II), and the corresponding local structures and compositions of ionic aggregates were investigated as a function of acid content and level of neutralization. Using X-ray scattering and scanning transmission electron microscopy, the sizes of ionic aggregates in Cu(II)-neutralized SMAA were found to be independent of acid content and neutralization level. The number density of ionic aggregates increased with acid content and neutralization level, but the increase is significantly less than expected for a fixed ionic aggregate composition. Electron spin resonance spectroscopy indicates three types of cation sites with corresponding relative population changing with acid content, which further indicates a compositional variation of ionic aggregates with neutralization level. The correlation between morphology and compositional evolution of the ionic aggregates will be discussed.

12:15PM V21.00006 Multiple Nanoscale Morphologies of Poly(Ethylene-co-Acryl Acid) Ionomers. CHRISTOPHER D. CHAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, TRAVIS W. RAUGHMAN, Macromolecular and Organic Chemistry, Technical University of Eindhoven, KATHLEEN L. OPPER, KENNETH B. WAGENER, Department of Chemistry, University of Florida, KAREN I. WINEY, Department of Material Science and Engineering, University of Pennsylvania — We have synthesized linear poly(ethylene-co-acrylic acid) (EAA) copolymers with precisely placed acid groups using ADMET (acyclic diene metathesis). In the acid form, the EAA copolymers with precisely placed acid groups exhibit the typical orthorhombic PE crystal structure along with a new layered structure. The layered structures coexist with the PE crystals and have spacings consistent with the separation between acid groups; at 9.5 mol% acid the layer-to-layer spacing is 2.53 nm. When these linear EAA copolymers are neutralized with zinc acetate in solution, high angle annular dark field scanning transmission electron microscopy (HAADF STEM) shows that the Zn-rich ionic aggregates decrease in size as the level of neutralization increases from 25% to 100%. X-ray scattering indicates that the cations decorate the acid-acid layered structure at low neutralization level, but eventually disrupt the layers at higher neutralization levels.

12:27PM V21.00007 Conduction, Ion Association and Dynamics in Polyethylene Oxide-based Polyester Ionomers1. DANIEL FRAGIADAKIS, SHICHEN DOU, RALPH COLBY, JAMES RUNT, Penn State University — A series of single-ion conducting PEO-based polyester copolymers is synthesized, containing different amounts of ionic sulfonate groups covalently attached to the polymer chains. The dynamics of the polymer chains and the mobile lithium cations is investigated using dielectric relaxation spectroscopy. A physical model of electrode polarization is employed to decompose dc conductivity into the contributions of the mobile ion concentration and ion mobility, and the physical meaning of these parameters and relation to literature results on similar systems is discussed. The segmental and local dynamics of the polymer chains is studied. We investigate both the modification of the dynamics due to the presence of the ionic groups, as well as the relation of chain motion to ion transport.

1Supported by the NSF Polymers Program and the Department of Energy

12:39PM V21.00008 Correlation between structure and conductivity in stretched Nafion. ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University — We have used coarse-grained simulation methods to investigate the effect of stretching-induced structure orientation on the proton conductivity of Nafion-like polyelectrolyte membranes. Recent experimental data on the morphology of ionomers describe Nafion as an aggregation of polymeric backbone chains forming elongated objects embedded in a continuous ionic medium. Uniaxial stretching of a recast Nafion film causes a preferential orientation of these objects in the direction of stretching. Our simulations of humid Nafion show that this has a strong effect on the proton conductivity, which is enhanced along the stretching direction, while the conductivity perpendicular to the stretched polymer backbone is strongly reduced. Stretching also causes the perfluorinated side chains to orient perpendicular to the stretching axis. The sulphonate multiplets shrink in diameter as the stretching is increased and show a spatially periodic ordering in their distribution. This in turn affects the distribution of contained water at low water contents. The water forms a continuous network with narrow bridges between small water clusters absorbed in head-group multiplets. We find the morphological changes in the stretched Nafion to be retained upon removal of the uniaxial stress.

1Work supported by DOE Grant DE-FG02-05ER46244

12:51PM V21.00009 Morphology study in block copolymer electrolytes. SCOTT MULLIN, NISITA WANAKULE, NITASH BALSARA, University of California, Berkeley — Poly(styrene-b-ethylene oxide)/lithium bis(trifluoromethane)sulfonimide (SEO/LITFSI) is of interest in battery applications since the doped PEO phase can conduct ions and the glassy PS phase can prevent dendrite growth upon recharging. It is believed that the LITFSI molecules are localized in the PEO microphases. Previous studies have shown that highly conducting electrolytes can be made from symmetric SEO copolymers. The purpose of this study is to explore the conductivity of asymmetric SEO copolymer systems doped with LITFSI. Our studies encompass both neat asymmetric SEO copolymers and SEO copolymers blended with PS homopolymers to separate the effects of architecture of the copolymer molecules and morphology adopted by the system in the melt state. Conductivity is measured by AC impedance, morphology is determined by small angle X-ray scattering, and crystallinity of the PEO chains is determined by differential scanning calorimetry. All samples were prepared in hermetically sealed sample cells in an Argon glovebox.

1:03PM V21.00010 Increased Water Retention in Polymer Electrolyte Membranes Assisted by Capillary Condensation. MOON JEONG PARK, NITASH P. BALSARA, Lawrence Berkeley National Laboratory, University of California, Berkeley — We establish a new systematic methodology for controlling the water retention of polymer electrolyte membranes. We show that block copolymer membranes with well-defined hydrophilic channels in the 2 to 5 nm range remain moist in a relatively dry environment (relative humidity = 50 %) up to temperatures as high as 90 °C. This retention of water leads to an increase in the overall conductivity with increasing temperature. Simple calculations suggest that capillary condensation is important at these length scales. The morphology of the hydrated membranes is determined by a combination of in-situ neutron scattering and cryogenic electron microscopy.

1:15PM V21.00011 Engineering polyelectrolyte multilayer structure at the nanometer length scale by tuning polymer solution conformation. SOHEIL BODDOHI, CHRISTOPHER KILLINGSWORTH, MATT KIPPER, Colorado State University — Chitosan (a weak polycation) and heparin (a strong polyanion) are used to make polyelectrolyte multilayers (PEM). PEM thickness and composition are determined as a function of solution pH (4.6 to 5.8) and ionic strength (0.1 to 0.5 M). Over this range, increasing pH increases the PEM thickness; however, the sensitivity to changes in pH is a strong function of ionic strength. The PEM thickness data are correlated to the polymer conformation in solution. Polyelectrolyte conformation in solution is characterized by gel permeation chromatography (GPC). The highest sensitivity of PEM structure to pH is obtained at intermediate ionic strength. Different interactions govern the conformation and adsorption phenomena at low and high ionic strength, leading to reduced sensitivity to solution pH at extreme ionic strengths. The correspondence between PEM thickness and polymer solution conformation offers opportunities to tune polymer thin film structure at the nanometer length scale by controlling simple, reproducible processing conditions.
complexes. This work is financially supported by the US-DOE grant DE-FG02-02ER46012.

Finally, we use a voltage dependent resonance-tunneling scheme to demonstrate a molecular switch made of F4TCNQ/6T charge transfer complexes. The charge transfer lead to the shift of HOMO and LUMO orbitals of the molecules in complexes with respect to the pure presented. The complexes are formed by self assembly of the electron donor RABE, Humboldt-Universität zu Berlin, Institut f. Physik, Newtonstraße 15, 12489 Berlin, Germany, S.-W. HLA, Ohio University, Physics and Astronomy Department, Athens, OH 45701, N. KOCH, J.P. RABE, Humboldt-Universität zu Berlin, Institut f. Physik, Newtonstraße 15, 12489 Berlin, Germany, S.-W. HLA, Ohio University, Physics and Astronomy Department, Athens, OH 45701 — A low temperature scanning tunneling microscope (STM) and spectroscopy study of organic charge transfer complexes is presented. The complexes are formed by self assembly of the electron donor- α-6T and the electron acceptor tetrafluorotetracyanoquinodimethane (F4TCNQ) on Au (111) surface. The formation of new hybrid molecular orbitals in CTCs is evident by STM imaging at different bias voltages as well as by differential conductance spectra. The charge transfer lead to the shift of HOMO and LUMO orbitals of the molecules in complexes with respect to the pure molecular orbitals. Finally, we use a voltage dependent resonance-tunneling scheme to demonstrate a molecular switch made of F4TCNQ/6T charge transfer complexes. This work is financially supported by the US-DOE grant DE-FG02-02ER46012.

Acknowledgment is made to the donors of Petroleum Research Fund, administered by the ACS, for support of this research.
12:27PM V22.00005 Correlating Structure and Conductivity of Pentathiophene Monolayers, BAS HENDRIKSEN, YABING QI, FLORENT MARTIN, Materials Sciences Division, Lawrence Berkeley National Laboratory, FRANK OGLETREE, The Molecular Foundry, Materials Sciences Division, Lawrence Berkeley National Laboratory, MIQUEL SALMERON, The Molecular Foundry and Materials Sciences Division, Lawrence Berkeley National Laboratory — Understanding the electrical conduction mechanisms in organic materials is important for the development of plastic and molecular electronics. The charge transport properties of conducting molecular layers are expected to strongly depend on the order of the layer and the conformation of the molecules. We used atomic force microscopy (AFM) to study and correlate the structural, mechanical and electrical properties to molecular monolayers of pentathiophene based molecules on solid substrates prepared by the Langmuir-Blodgett technique. The molecular monolayers consist of two phases: one phase of compact micromer size-flowered islands and a phase with less order and a high density of holes. We found that the perpendicular conductivity, i.e. through the monolayer sandwiched between the conductive AFM probe and the conductive substrate, is more than 5 times higher on the well-ordered island phase. This shows that the molecular lattice order has a significant effect on the electronic properties.

12:39PM V22.00006 Direct measurement of photomechanical switching cross-sections of single-molecules on a surface, JONGWON CHO, MATTHEW J. COMSTOCK, NIV LEVY, LUIS BERTIL-BAUTISTA, FRANK LAUTERWASSER, JEAN M. J. FRECHET, MICHAEL F. CROMMIE, University of California at Berkeley — The photomechanical switching of photoactive molecules in solution strongly depends on the wavelength of light. This dependence is crucial to reliably control the photomechanical state of target molecules. Recently, reversible photomechanical switching of individual azobenzene molecular derivatives on the Au(111) surface has been reported for one particular wavelength of UV illumination [1]. To further understand this process and its possible applications in future nanotechnologies, we have investigated photomechanical switching rates and saturation behavior for azobenzene molecular derivatives at a surface under optical stimulation at different wavelengths. Using single-molecule-resolved scanning tunneling microscopy, we have determined both the forward and reverse photomechanical molecular switching cross-sections at different wavelengths. In a dramatic departure from solution-based environments, visible light does not efficiently reverse the photoreaction. [1] Matthew J. Comstock, Niv Levy, Armen Kirakosian, Jongwoon Cho, Frank Lauterwasser, Jessica H. Harvey, David A. Strubbe, Jean M. J. Fréchet, Dirk Trauner, Steven G. Louie, and Michael F. Crommie, Phys. Rev. Lett. 99, 038301 (2007)

12:51PM V22.00007 Many-body treatment of quantum transport through single molecules, JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona — We investigate multi-terminal quantum transport through single molecules including intramolecular correlations exactly by using the nonequilibrium Green function approach, but treating the lead-molecule coupling perturbatively via a Dyson expansion [1]. We find many transport features which are not accessible via mean-field approaches such as Coulomb blockade steps and an incipient Hubbard-Mott insulator gap. We also calculated the thermopower exactly and in find, in accordance with recent experimental [2] and theoretical reports, that the transport in this junction is dominated by holes (p-type). This result allowed us to then extract the remaining free parameter, the lead-molecule coupling Γ. The resulting nonlinear I-V curve was found to be in good quantitative agreement with experiment. Finally, we calculated the differential conductance as a function of gating and bias potential to construct a full molecular ‘Coulomb diamond’.


1:03PM V22.00008 Single molecule characterization with well-defined contacts, ALEX NEUHAUSEN, FRANK JAECKEL, JEREMY HIATT, JOSEPH SULPIZIO, DAVID GOLDBADER-GORDON, CHRIS CHIDSEY, W. E. MOERNER, ZHENAN BAO, Stanford University — We demonstrate a novel method to reliably achieve ohmic contact to single molecules in a geometry that allows for simultaneous transport measurements and Raman spectroscopy. We achieve this by lithographically defining gold contacts to a structure composed of a single molecule bridging a pair of gold nanoparticles. The transport measurements indicate negligible resistance from the contacts as compared to the single molecule behavior, and the Raman spectroscopy benefits from strong field enhancement between the two nanoparticles. We prove the presence of single molecules with both stoichiometric and disordered structures. The transport measurements indicate negligible resistance from the contacts as compared to the single molecule behavior, and the Raman spectroscopy benefits from strong field enhancement between the two nanoparticles. We prove the presence of single molecules with both stoichiometric and disordered structures. This work was supported by an NSF NIRT grant.

1:15PM V22.00009 Transport Fluctuations in Metal-Molecule Junctions, JONATHAN MALEN, KANHAY-ALAL BAHETI, PETER DOAK, RACHEL SEGALMAN, ARUN MAJUMDAR, UC Berkeley — Thermopower of metal-molecule junctions is an alternative spectroscopic technique for determining the electronic structure of single-molecules. We have measured the thermopower of such molecular junctions. Temperature bias applied between gold contacts across the bridging molecules generates a thermoelectric voltage. Hitherto, the statistical analysis of the data from both thermopower and conductance measurements has focused on the histogram peaks rather than the spread of the data. We find that the full width half maximums (FWHM) of the voltage histograms are finite at zero temperature bias and increase in proportion to the temperature bias. Johnson Noise is the most likely cause of the zero bias FWHM, and its magnitude is thereby related to the junction conductance. We find that the FWHM of the voltage histograms are finite at zero temperature bias and increase in proportion to the temperature bias. Johnson Noise is the most likely cause of the zero bias FWHM, and its magnitude is thereby related to the junction conductance. We find that the FWHM of the voltage histograms are finite at zero temperature bias and increase in proportion to the temperature bias. Johnson Noise is the most likely cause of the zero bias FWHM, and its magnitude is thereby related to the junction conductance. For 1,4-Benzenedithiol (BDT) the junction conductance associated with the zero bias FWHM is 0.02 eAu, in close agreement with prior conductance measurements of BDT. The dependence of FWHM on temperature bias may provide further insight to the origin of stochastic fluctuations in metal molecule junctions.

1:27PM V22.00010 Electronic transport through single-molecule- and monolayer-based molecular junctions, LUIS AGAPITO, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, Florida 32611 — We report our development for calculating tunneling electronic transport through molecular junctions, which are composed of two contact leads and the active device in between. The surface Green’s function of the contact leads is obtained following a non-iterative, exact procedure using ab initio data computed with the same level of theory and localized basis set than those used for the active device*. In a 1-dimensional in-wire setting, we describe the electrical switching performance of a single oligo-phenylene-ethynylene molecule connected to graphene-nanoribbons leads. Moreover, in a more realistic 2-dimensional setting, such as the case of self-assembled molecular monolayers, the method is extended to include intermolecular and packing-density effects. * Agapito, L. A.; Cheng, H. P. Journal of Physical Chemistry C 2007, 111, 14266.

[1] We acknowledge the U.S. Department of Energy under contract no. DE-FG02-02ER45995.

1:39PM V22.00011 ABSTRACT WITHDRAWN —
1:51PM V22.00012 Substrate-Dependent Electronic Behavior of Polydiacetylene Nanowires
RAJIV GIRIDHARAGOPAL, K. F. KELLY, Rice University — Scanning tunneling microscopy (STM) has been used to study individual polydiacetylene (PDA) nanowires. STM analysis of PDA nanowires on different substrate electrode materials at varying sample bias voltage conditions reveals interesting substrate-dependent effects. PDA nanowires were formed on both graphite and molybdenum disulfide (MoS₂) substrates. Interestingly, the nanowires on graphite appear with different topographic heights depending on the substrate bias voltage, and the height varies substantially with respect to voltage polarity. A similar effect is observed on MoS₂ at negative sample bias voltages, except that the nanowires are almost twice as tall on MoS₂. Even more intriguing is that at positive sample bias voltage conditions, the nanowires on MoS₂ are invisible in all STM images. A comparison of these voltage-dependent effects points to a strong influence of the substrate electrode material on the electronic behavior of these polymer nanostructures. The results reported here have implications for recently-demonstrated technologies such as monolayer PDA transistors and PDA-based organic solar cell devices as well as potential molecular electronic systems.

2:03PM V22.00013 Organic memory devices using the negative differential resistance effect
R. OSTERBACKA, J.K. BARAL, H.S. MAJUMDAR, F. JANSSON, Center for Functional Materials and Department of Physics, Abo Akademi, Finland, A. LAHJO, R.H.A. RAS, J. RUSCHE, O. IKKALA, Department of Engineering Physics and Mathematics and Center for New Materials, Helsinki University of Technology, Finland, H. JIANG, E. KAUPPINEN, VTT Biotechnology, Finland — Of all the organic memory devices reported so far the ones having the negative differential resistance (NDR) is the best in terms of yield, reproducibility and repeatability. We have observed two different kinds of NDR in nanoparticle based organic memory devices. One is the memory-NDR which follows the observation in SiO₂ devices [Simmons et. al. Proc. R Soc. Lond. Ser. A 301 (1967)][7]. Here the I-V characteristics track different paths based on device history. The second type is the tunneling-NDR, where the I-V curves always trace the same path, irrespective of the history. This behavior is similar to the one observed in resonant tunnel diodes and multiple tunneling is the explanation. We have performed a multitude of optical and electrical experiments and clarified the influences of morphology on the complex and interesting device performance observed in this new class of organic electronic devices.

Thursday, March 13, 2008 11:15AM - 2:15PM –
Session V23 DMP GMAG: Focus Session: Charge/Orbital Ordering in Complex Oxides Morial Convention Center 215

11:15AM V23.00001 Evolution of the ‘Orbital Peierls State’ with doping
C. ULRICH, G. KHALIJULLIN, B. KEIMER, Max-Planck-Institute FKF; Stuttgart, Germany, M. REEHUIS, HMI, Berlin, Germany, K. SCHMALZL, A. IVANOV, ILL, Grenoble, France, K. HRADIL, FRM II, Munich, Germany, J. FUJIOKA, Y. TOKURA, University of Tokyo, Japan — Orbital degrees of freedom play an important role in the physics of strongly correlated electron systems. Our extensive investigation of insulating vanadates by neutron scattering has led to the discovery of an unusual magnetic ground state. YVO₃ exhibits two magnetic phases, a C-type phase below 116 K and 77 K and a G-type phase below 77 K. While the magnetic properties of the G-type phase are in accordance with standard theories, the C-type phase shows highly unusual static and dynamic spin correlations. Based on the idea of orbital fluctuations we were able to identify this phase as a theoretically predicted ‘orbital Peierls state’[1]. Neutron scattering experiments on Y₁₋ₓCaₓVO₃ show that the C-type phase, i.e. the ‘orbital Peierls phase’, is stabilized upon doping, while the orbitally ordered G-type phase is quite unstable and disappears at x = 2%. Furthermore, with doping this phase also exhibits a highly unusual spin wave dispersion. These leads us to the conclusions, that the ‘orbital Peierls state’ becomes more robust with Ca-doping, whereas the formerly well defined G-type phase exhibits a more complex behaviour, probably as a consequence of an increase in orbital fluctuations. [1] C. Ulrich et al., PRL 91, 257202 (2003).

11:27AM V23.00002 Magnetic interactions and orbital physics in RVO₃ perovskites
J.-Q. YAN, Ames Laboratory, Ames, IA 50011, S. CHANG, C. BROWN, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, M. HEHLEN, F. TROUW, LANSC, Los Alamos National Laboratory, Los Alamos, NM 87545, R.J. MCQUEENEY, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA 50011 — We have performed inelastic neutron scattering study on high quality YVO₃ and LaVO₃ powders. The magnetic interactions determined from the scattering spectra for YVO₃ agree with a previous single crystal study. [1] For LaVO₃, a −Jab > Jc is in sharp contrast to the Jc > Jab in the C-type magnetically (C-AF) ordered state of YVO₃. The mechanism that greatly suppresses Jab in C-AF state of YVO₃ will be discussed together with thermal conductivity [2] and Raman spectroscopy [3] results.

11:39AM V23.00003 Pressure-temperature phase diagram for orbital and spin states in RVO₃ (R=Y,Tb)
DAISUKE BIZEN, KEISUKE NAKATSUKA, TETSUYA MURATA, HIRONORI NAKAO, KAZUAKI IWASA, YOUICHI MU-RAKAMI, Tohoku University, TOYOTAKA OSKABE, JAEA, SHIGEKI MIYASAKA, Osaka University, YOSHINORI TOKURA, University of Tokyo, CERC-AIST — Perovskite-type vanadium oxides RVO₃ (R=Y, La-Lu) show various physical properties coupled with the orbital and spin states. Orbital ordered states of V 3d⁵ in YVO₃ have been systematically investigated by X-ray scattering technique under high-pressure and low-temperature (HP-LT). The pressure-temperature phase diagram for the orbital state was clearly determined from the crystal parameters, i.e. the lattice constants and the reflection conditions. It indicates that the C-type orbital ordering (C-OO) is stabilized as compared to the G-type orbital ordering (G OO) by applying hydrostatic pressure. Based on the result, we succeeded in controlling the ground state of 3d-orbital in TbVO₃ from G-OO to C-OO by applying pressure. The spin state coupled with the orbital was also studied by neutron scattering under HP-LT. It elucidated that the magnetic ground state changed from the C-type spin ordering to the G-type one. This result indicates the strong coupling between orbital and spin states.

11:51AM V23.00004 Stabilization of Charge Ordering by Magnetic Exchange
ROBERT MCQUEENEY, Iowa State University/Ames Laboratory — The magnetic exchange energies in charge ordered La₃Sr₂Fe₃O₈ (LSFO) and its parent compound LaFeO₃ (LFO) have been determined by inelastic neutron scattering. In LSFO, the measured ratio of ferromagnetic exchange between Fe³⁺-Fe³⁺ pairs (J_F) and antiferromagnetic exchange between Fe³⁺-Fe⁵⁺ pairs (J_AF) fulfills the criterion for charge ordering driven by magnetic interactions (J_F/J_AF > 1). The 30% reduction of J_AF as compared to LFO indicates that doped holes are delocalized, and charge ordering occurs without a dominant influence from Coulomb interactions.

¹ Ames Laboratory is supported by USDOE under Contract No. W-7405-ENG-82.
12:27PM V23.00005 Electronic Raman Scattering in Magnetite: Spin vs. Charge gap

12:39PM V23.00006 Electrically-driven phase transition in magnetite nanostructures

12:51PM V23.00007 Pressure-Induced Intermetallic Valence Transition in BiNiO₃

1:03PM V23.00008 Phonon Anomaly across Charge/Orbital Ordering Transition in Pr₀.65Ca₀.35MnO₃

1:15PM V23.00009 Charge Ordering in Half-Doped Manganites: Small Charge Disproportion and Leading Mechanisms

1:27PM V23.00010 Orbital ordered phases of Mn₃O₄ and MnV₂O₄ investigated by NMR

1:39PM V23.00011 Orbital Order and Metal-Insulator Transition in PbRuO₃

[1] This work was supported by the Alexander von Humboldt Foundation, Research Corporation Cottrell College Science Award # CC 6130/5742 and Petroleum Research Fund Award # 40926-GB10.
The conduction mechanism mediated by the LUMOs of the C$_{60}$ molecule is revealed. Due to the bias effect on the LUMO alignment, negative differential resistance (NDR) is observed in both two- and three-terminal devices at a very low bias. Since the LUMOs can be easily modified by molecular adsorption, the NDR position is tunable and can be used in sensor applications without the need for specific molecular receptors.

1:51PM V23.00012 Incommensurate Magnetic Structure of ZnCr$_2$Se$_4$ and ZnCr$_2$S$_4$. FABIANO YOKAIKIYA, Hahn-Meitner-Institut, Hahn-Meitner-Institut, 100 Glenicker str, Berlin, Germany, HELOISA NUNES BORDALLO, DIMITRI ARGYRIOU, Hahn-Meitner-Institut, 100 Glenicker str, Berlin, Germany, A KRIMMEL, A LOIDL, V TSURKAN, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — Recent studies of chalcogenide chromium spinels have shown a coupling between ferroelectricity and magnetism. The motivation of this work is to determine the magnetic ground state, (including its symmetry properties), to comprehend the coupling of magnetic and ferroelectric order parameters in the spinels ZnCr$_2$Se$_4$ and ZnCr$_2$S$_4$. The incommensurate magnetic structures through the Néel transition in these systems have been studied by high-resolution powder neutron diffraction. Below $T_N$ ($\sim$22K), for both cases, the magnetic structure is described as ferromagnetic layers in the ab-plane stacked in a spiral arrangement along the c-axis with a propagation vector $\mathbf{k} = (0.0, 0.46)$. In ZnCr$_2$Se$_4$ and ZnCr$_2$S$_4$, the magnetic phase transition is of first order. Therefore to use the irreducible co-representation theory, for symmetry analysis, the magnetic phase is described by a linear combination of irreducible representations. In this talk we present results of Rietveld analysis on the magnetic and crystal structure through the magnetic transition.

2:03PM V23.00013 ABSTRACT WITHDRAWN —

Thursday, March 13, 2008 11:15AM - 1:51PM — Session V24 DMP: Focus Session: Transport in Nanostructures VII: Si Interfaces and Carbon

11:15AM V24.00001 Leakage current in deca-nano MOSFET by surface state hopping$. HASSAN RAZA, EDWIN KAN, School of Electrical and Computer Engineering, Cornell University Ithaca NY 14853 — Si surface states have been a topic of recent study [Nature 439, 703 (2006), PRB 76, 045308 (2007)]. In this work, we present transport calculations through these surface states, which result in a two-dimensional system. Among the systems being considered are: (1) $\pi$ and $\pi^*$ states on Si(100)/(2x1) surface with asymmetric dimer reconstruction, and (2) dangling bond wires along and perpendicular to the dimer row direction. Previously, we have reported the electronic structure of these systems in PRB 76, 045308 (2007). Here, we show that these states can give rise to significant current densities and hence may contribute to subthreshold leakage. Furthermore, the transport depends on the location of Fermi level with respect to the band edge and hence on the Fermi level pinning. We use EHT (extended Huckel theory) for the electronic structure and NEGF (non-equilibrium Green's function) formalism for the mean-field quantum transport. EHT has been applied to Si bulk and surfaces and gives quantitative agreement with experiments, e.g. band gap and band dispersions.

$^1$The work is supported by National Science Foundation (NSF) and by Nanoelectronics Research Institute (NRI) through Center for Nanoscale Systems (CNS) at Cornell University.

11:27AM V24.00002 Tunneling properties of ultra-thin SiO$_2$ barriers: a first-principles study. EUNJUNG KO, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul, Korea — We performed first-principles simulations of the electron tunneling through ultra-thin SiO$_2$ barriers in Si(100)/SiO$_2$/Si(100) structures. The atomic structures of the Si/SiO$_2$ interfaces are generated by considering various silicon suboxide states observed in photoemission studies. For comparison, we also consider sharp Si/SiO$_2$ interfaces with dangling bonds. For each atomic structure, the tunneling conductance is calculated by a first-principles scattering-state method based on the ab-initio pseudopotentials and the density functional theory within the local density approximation. As a result we obtained the dependence of the tunneling probabilities on the oxide thickness and on the interfacial structures. Effects of the dangling bonds on the tunneling probabilities will also be discussed. Computational resource for this work is provided by KISTI under the 8th Strategic Supercomputing Support Program.

11:39AM V24.00003 C$_{60}$-based devices: large scale simulations and design. X. H. ZHENG, W. LU, T. A. ABTEW, NC State University, V. MEUNIER, Oak Ridge National Laboratory, J. BERNHOLC, NC State University — C$_{60}$ is one of the most promising building blocks in the design of molecular devices, due to its spherical symmetry and structural reproducibility. In this work, the electron transport properties of two- and three-terminal devices built of C$_{60}$S are investigated. The C$_{60}$S are connected by alkane chains and then sandwiched between aluminum nanowires. The calculations are carried out using a massively parallel real-space multigrid O(N) implementation of density functional theory. The conductance and nonlinear I-V characteristics are evaluated by the LUMOs of the C$_{60}$ molecules is revealed. Due to the bias effect on the LUMO alignment, negative differential resistance (NDR) is observed in both two- and three-terminal devices at a very low bias. Since the LUMOs can be easily modified by molecular adsorption, the NDR position is tunable and can be used in sensor applications without the need for specific molecular receptors.

11:51AM V24.00004 Quasiparticle Gaps of Nanostructures Weakly-Coupled to their Environments: The Case of C60/Metal Interfaces$. JAY SAU, Department of Physics, U C Berkeley, Material Science Division, LBNL, JEFFREY NEATON, Molecular Foundry, LBNL, HYOUNG-JOON CHOI, Department of Physics and IPAP, Yonsei University, Korea, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, U C Berkeley, Material Science Division, LBNL — A new approach based on density functional theory is developed to calculate charging energies and quasiparticle energy gaps of molecular systems weakly-coupled to an external environment. The approach is then applied to the case of a C60 molecule adsorbed on the Au(111) and Ag(100) surfaces. For C60/Au(111), the calculated quasiparticle gap is reduced by 2.34 eV relative to the gas-phase, consistent with recent experiments. For the more strongly-coupled C60/Ag(100) system, the predicted gap is also reduced, but differs from experiment by 0.5 eV. The discrepancy is identified as being due to screening due to charge transferred from the metal to the molecule and is resolved by solving an effective Anderson Hamiltonian within the GW approximation for the carriers in the HOMO and LUMO states, which results in an extra renormalization of the gap for the Ag(100) case.

$^2$This work was supported by NSF Grant No. DMR07-05941 and by DOE under Contract No. DE-AC02-05CH11231. Computational resources were provided by Indiana University, SDSC, NERSC, TACC.

12:03PM V24.00005 ABSTRACT WITHDRAWN —
12:15PM V24.00006 Electron-phonon scattering effects on transport properties of carbon nanotube devices using time-dependent wave-packet approach. HIROYUKI ISHII, National Institute of Advanced Industrial Science and Technology (AIST), NOBUHIKO KOBAYASHI, University of Tsukuba, KENJI HIROSE, NEC Corporation — Single-walled carbon nanotubes have been expected as nanoscale electronic devices, because the nanotubes are very good conductors exhibiting ballistic transport properties. However, the electronic current is saturated by the electron-phonon coupling. To realize the application of carbon nanotube devices, understanding of the scattering mechanism is required. We investigated the electron-phonon coupling effect on the transport properties of the nanotubes with micron order channel length, using the time-dependent wave-packet approach under a tight-binding approximation [1]. The vibrational atomic displacements in real space are introduced through the time-dependent Schrödinger equation and obtained the diffusion coefficients of the electronic wave packets. From these data, we can extract the mean free path and conductance. We clarified the difference of the phonon scattering effects on the conductance of the metallic nanotube and the semiconducting one. Furthermore we investigate the channel length dependence of resistance from ballistic to diffusive transport characteristics. [1] S. Roche et al., PRL 95 (2005) 076803

12:27PM V24.00007 ABSTRACT WITHDRAWN –


12:51PM V24.00009 Multiple Well Structures of Graphene1,2. HALDUN SEVINCI, Department of Physics, Bilkent University, Ankara 06800, Turkey, MEHMET TOPSAKAL, SALIM CIRACI, UNAM-Institute for Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey. — Based on first-principles calculations we predict that periodically repeated junctions of graphene ribbons of different widths form a multiple-well graphene structure. In such structures, the energy bands of graphene are discretized into unique, size-selected confined states. The width of the well as well as the bad gap, even the magnetic ground state for specific superlattices are modulated in direct space. Orientation of constituent ribbons, their width and length, the symmetry of the junction and their functionalization by adatoms are structural parameters to engineer electronic and magnetic properties of the quantum structure. Not only the size modulation, but also composition modulation such as the heterojunction of BN in honeycomb structure and graphene gives rise to confined states. Devices made from these graphene quantum structures display negative differential resistance. 1Part of the computations has been carried out by using UYBHM at Istanbul Technical University.

1:03PM V24.00010 Direct measurement of electric-field-screening length in thin graphite film. H. MIYAZAKI, RIKEN and JST-CREST, K. TSUKAGOSHI, RIKEN, AIST, and JST-CREST, S. ODADA, Y. AYOAGI, RIKEN, Tokyo TECH, and JST-CREST, T. SATO, S. TANAKA, H. GOTO, A. KANDA, Y. OOTUKA, Univ. of Tsukuba and JST-CREST — Electric-field-screening length in thin graphite film has been clarified by means of dual gated method. Sandwich type device structure which two gate electrodes are situated over and beneath a graphite film was constructed with Al top electrode. The Al electrode naturally generates thin gate insulator at graphite/Al interface, which enables extremely low voltage swing. The two systems are studied to determine how a chemical absorbate and linker influence transport through metallic CNTs. The first system consists of a stand alone metallic CNT with a single oxygen adsorption site, matching a proposed final chemical process for a HNO3 oxidation and reduction process. The second system consists of a CNT-Amide-(CH2)6-Amide-CNT structure in which both CNTs are metallic. Transmission calculations, using our DFT (FIREBALL)-NEGF code show that the amide linker suppresses transmission compared to a direct CNT-polyene linkage studied in [3]. 1. B. R. Goldsmith, et. al., Science, 315, 77 (2007). 2. X. Guo, et. al. Science, 311, 356 (2006). 3. N. Bruque, et. al. Phys. Rev. B, 76, 205322 (2007).

1:15PM V24.00011 Surface Potentials and Layer Charge Distributions in Few-Layer Graphene1. SUJIT DATTA, DOUGLAS STRACHAN, EUGENE MELE, A.T. CHARLIE JOHNSON, Department of Physics and Astronomy, University of Pennsylvania — Elucidating the electronic interaction between an insulating substrate and few-layer graphene (FLG) films is crucial for graphene device applications. We have performed electrostatic force microscopy (EFM) of FLG films. Our measurements reveal that the FLG surface electrostatic potential increases with film thickness, approaching a ‘bulk’ value for samples with five or more graphene layers - contrasting sharply with behavior expected for conventional conducting or semiconductor films. This is in quantitative agreement with the analytic predictions of a nonlinear Thomas-Fermi theory of the interlayer screening by the few-layer graphene's relativistic low energy charge carriers. Furthermore, our measurements are able to resolve previously unseen electronic perturbations extended along crystallographic directions of stressed samples, likely resulting from long-range atomic defects. 1Research supported by Nano/Bio Interface Center through the National Science Foundation NSEC DMR-0425780; the JST DTRA and the Army Research Office Grant # W911NF-06-1-0462; and Department of Energy Grant # DE-FG02-06ER46118.

1:27PM V24.00012 Valley contrasting physics in graphene: magnetic moment and topological transport. QIAN NIU, DI XIAO, WANG YAO, The University of Texas at Austin — We investigate physical properties that can be used to distinguish the valley degree of freedom in graphene systems with broken inversion symmetry. We show that the pseudospin associated with the valley index of carriers has an intrinsic magnetic moment, in close analogy with the Bohr magneton for the electron spin. There is also a valley dependent Berry phase effect that can result in a valley contrasting Hall transport, with carriers in different valleys turning into opposite directions transverse to an in-plane electric field. These effects can be used to generate and detect valley polarization by magnetic and electric means, forming the basis for the so-called valleytronics applications.

1:39PM V24.00013 Quantum transport of 2D Dirac fermions: the 2D symplectic symmetry class of Anderson localization and the Z2 topological term. SHINSEI RYU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CHRISTOPHER MUDRY, Paul Scherrer Institute, Switzerland, HIDEAKI OBUSE, AKIRA FURUSAKI, RIKEN, Japan — We discuss the quantum transport of the 2D non-interacting Dirac Hamiltonian, which, underlies theoretical descriptions of graphene and surface states of 3D Z2 topological insulators. For a random scalar potential type disorder, a Z2 topological term is derived in the non-linear sigma model encoding the physics of Anderson localization in the symplectic symmetry class. Unlike the Pruisken term (Chern integer) in the IQHE, the Z2 topological term cannot be expressed, in general, as an integral of a local quantity, but as a sign of the Pfaffian of a family of Dirac operators. The Z2 topological term has a significant effect on the renormalization group flow of the conductance.
11:15AM V25.00001 A model for glass transitions in polymer thin films.¹ JANE LIPSON, Dartmouth
College — Polymeric materials formulated as thin films can exhibit glass transition temperatures which are significantly shifted relative to bulk values. Depending on whether the film is supported (on a substrate) or freely-standing the temperature shift can go in different directions relative to the bulk. For all films the magnitude of the shift depends on film thickness. For supported films the shift appears to depend on substrate-polymer interactions, while for free-standing films there is a striking dependence on molecular weight. Experimental data published over the last five years have included some elegant and intriguing results which provide a significant challenge for those wishing to understand these phenomena. In this talk a model that predicts glass transitions in both free-standing and supported films will be presented and tested against extant data. Ideas for future experiments will also be discussed.

¹Work done in collaboration with Scott Milner, ExxonMobil Research and Engineering.

11:51AM V25.00002 Creating defect free structures by directed photochemical reaction in a ternary phase separating system. PRATYUSH DAYAL, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — We present a technique to create long range ordered structure in photosensitive reaction-diffusion systems. Our approach utilizes a reversible photochemical reaction between species A and B in a ternary immiscible ABC blend to yield a defect-free arrangement of phase separated ABC domains. The process essentially consists of two steps. First, the sample is irradiated by virtue of masks creating an illumination pattern which allows the migration of AB components to the covered regions at the expense of the C component. As a result the C component is pinned onto the irradiated regions which in turn leads to pinning of AB domains thereby creating a long range order in the system. Second, the masks are completely removed and whole sample is irradiated uniformly. In this case, the system evolves into a distinctly different ordered structure. The ordering of the system, either before or after removal of the mask, can be locked in by quenching the system at appropriate temperature. Simulation studies reveal that the ordering can be controlled by changing the initial concentration of the blend as well as by varying size and arrangement of the holes in the mask. The defect free morphology has been demonstrated for rectangular, hexagonal and parallel arrangement of the masks.

12:03PM V25.00003 Entropic Effects in the Phase Behavior of Athermal Nanoparticle/Homopolymer Thin Film Mixtures , LUCIANA MELI, ABRAHAM ARCEO, PETER GREEN, University of Michigan — The phase behavior of an athermal nanoparticle/polymer mixture, composed of polystyrene-coated gold nanoparticles embedded in polystyrene thin film hosts, was examined. It is shown that the spatial distribution of nanoparticles is readily tailored through control of: the grafting density of the brush, the length of both grafted and free chains, and the relative size of the nanoparticles in comparison to the size of the polymer melt chains. The distribution of nanoparticles within the polymer host, including a surface-induced phase separation, may be understood as a balance between the conformational entropy of the polymer chains, which is compromised when the chains have to stretch around the nanoparticles and penetrate their brush, and the translational entropy of the nanoparticles, which favors their homogeneous distribution. This is the first report that systematically studies the entropic effects that lead to surface phase transitions in polymer/nanoparticle thin film mixtures. Our results may also prove helpful in understanding nanofiller dispersion in analogous bulk mixtures.

12:15PM V25.00004 Mechanism of Interfacial Instability in Thin Polymer Film in Controlled Solvent Atmosphere , PARMANAMOKARIAN-TABARI, JONATHAN. R. HOWSE, SASHA Y. HERIOT, MARK GEGHEGEGH, RICHARD A.L. JONES, Department of Physics and Astronomy, The University of Sheffield, Sheffield, S3 7RH, UK — Thin films of immiscible polymers made by spin coating have potential for many practical applications like field-effect transistors, LEDs and photovoltaic devices. We have developed a technique based on small angle light scattering and reflectivity to study the process of phase separation in spin cast films in situ during formation. Previous experiments proposed formation of a transient wetting layer which is followed by interfacial instability and leading to lateral phase separation. In our recent work the origin of this instability has been studied. Experiments have been designed to test the Marangoni instability by spin coating the PS/PMMA film in a controlled toluene vapour atmosphere. A fast evaporation rate leads to laterally phase separated structure whereas slow evaporation lowers the solvent gradient inside the film and leads to a self stratiﬁed structure. By comparing the data to a model a better understanding of film evolution has been established.

12:27PM V25.00005 Spanning Trees and the Dynamics of Compact Polymers , ARMIN RAHMANI, ANDREA VELENICH, CLAUDIO CHAMON, Physics Department, Boston University — We introduce a lattice model for a compact loop polymer conﬁned to a two-dimensional box. A mapping to spanning trees on a square lattice we calculate the partition function and the energy of the system as a function of temperature, bending rigidity and elasticity of the polymer. We study the dynamics of the system using a kinetically constrained model whose elementary moves consist of polymer ﬁnger ing or, in the language of the spanning trees, local bond ﬂips taking place at the leaves of the tree. We study, through Monte-Carlo simulations, the time dependence of the energy and the number of leaves in the system when quenched from inﬁnite temperature to various ﬁnite temperatures. We ﬁnd that for temperatures above a critical value, these observables monotonically decay to their equilibrium values whereas, for lower temperatures, a broad non-equilibrium plateau emerges.

¹NSF Grant DMR-0403997

12:39PM V25.00006 Upper Limit of Superheating in Polymer Crystals Revealed from Linear Heating Covering Seven Orders of Magnitude in Heating Rate , CHRISTOPH SCHICK, University of Rostock, Germany, ALEXANDER MINAKOV, General Physics Institute, Moscow, Russia, ANDREAS WURM, University of Rostock, Germany — We report about superheating of polymer crystals on linear heating covering the scanning rate range from 0.02 to 1,000,000 K/s. Results obtained by super-fast scanning calorimetry using a thin film sensor [1] are combined with results from DSC. On slow heating semicrystalline polymers tend to recrystallize (reorganize) significantly fast. From previous measurements the onset of melting of isothermally crystallized samples can be attributed to the rising flank of the first melting peak, which is often described by the power law of superheating:

\[ T \sim (T - T_{\alpha})^\alpha \]

with \( \alpha < 0.2 \), which does not correspond to the heat transfer but rather to a nucleation process [2]. At high heating rates superheating saturates. The power law behavior and the saturation of superheating will be discussed. 1. A.A. Minakov, C. Schick, Rev. Sci. Instrum. 78 (2007) 073902. 2. A.A. Minakov, A. Wurm, C. Schick, Europ. Phys. J. E, 23 (2007) 43.
12:51PM V25.00007 Molecular simulation of crystal nucleation of an n-alkane, PENG YI1. GREGORY RUTLEDGE2. Massachusetts Institute of Technology — We report the results of molecular simulations to study crystal nucleation of n-octane from the melt. A realistic united atom force field was employed for n-octane. The melting behavior was first determined by ramping temperature in a set of Monte Carlo simulations. The adiabatic nucleation trajectory was then sampled using the umbrella sampling technique with a set of proposed global and local order parameters, and analyzed for selection of best order parameter. The transition state ensemble has been verified by molecular dynamics simulation. The structure of critical nuclei in the nucleation process is analyzed and the effect of intermediate phases discussed.

1Department of Physics
2Department of Chemical Engineering

1:03PM V25.00008 Entropically Driven Layering Near a Substrate: A Fluids DFT Study, ERIN MCGARRITY, Michigan State University, AMALIE FRISCHKNECHT, Sandia National Laboratory, MICHAEL MACKAY, Michigan State University — We employ a fluids density functional theory to study the phase behavior of athermal polymer/nanoparticle blends near a hard substrate. These blends exhibit two types of first order, entropically driven layering transitions. In the first type of transition, the nanoparticles order to form a layer which is a fixed distance from the surface. The structure and location of this layer depends on nanoparticle radius. In the second type of transition, which occurs at melt-like densities, the nanoparticles and polymers form lamellar structures which resemble colloidal crystals. We examine the effects of packing density, chain length and nanoparticle radius on the system and show that the transitions are first order. In addition we show that the crystalline phase is nucleated by the presence of the surface. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:15PM V25.00009 Properties of Ferroelectric Polyvinylidene fluoride-co-trifluoroethylene Nanorods, JODIE LUTKENHAUS, Yale University, THOMAS RUSSELL, University of Massachusetts Amherst — Ferroelectric and piezoelectric nanorods of polyvinylidene fluoride (PVdF) are potential candidates for sensing mechanical stimuli on the nano-scale. Untreated PVdF tends to crystallize in a non-ferroelectric (α) phase. PVdF-co-trifluoroethylene (PVdF-TrFE), on the other hand, readily crystallizes into the ferroelectric (β) phase; however, the structure and properties can be significantly influenced by confinement. Here, the creation of PVdF-TrFE nanorods (dia. = 15 to 200 nm) using anodized aluminum oxide membranes was investigated. The crystallization behavior and the Curie transition (ferro- to paraelectric phase) were studied. Changes in structure and phase were investigated by X-ray diffraction (XRD) and differential scanning calorimetry (DSC). The effects of electrical poling, which increases dipole-orientation within the ferroelectric phase, are discussed.

1:27PM V25.00010 Thermodynamics and Kinetics of Crystallization of Flexible Molecules, BERNHARD WUNDERLICH, Retired — The crystallization of a single atom (as in a metal) is a one-step transfer across the liquid-crystal interface. A flexible chain molecule of n segments needs considerably more steps. A simple description gives it (n - 2) steps. The melting temperature of pentamethylene, i.e., for pentamethylene C5H102 111,000, but only one conformation in the crystal, making the crystallization a multi-step process. At what length are there too many steps to allow the crystallization to be reversible? How can one describe phase separation for flexible molecules containing segments of different chemical nature? How do random segments of different nature and precisely spaced segments of different nature influence the phase separation on crystallization? How is reversible crystallization influenced by chain folding and crystal perfection in the solid state? Some of these old questions can now be answered by temperature-modulated differential scanning calorimetry of precisely made molecules of different length and copolymerized structure.

1:39PM V25.00011 UV-convergent One-loop Theory of Binary Homopolymer Blends, JIAN QIN, FRANK BATES, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — We analyze the effects of long wavelength composition fluctuations in binary homopolymer blends. We use a generalization of Wang’s theory [1], in which all dependence upon short-wavelength structure is absorbed into a renormalization of an effective χ parameter χ e and of statistical segment lengths. The theory allows us to calculate the collective correlation function S(λ), single chain correlation functions, and the free energy density in homogeneous mixtures. The same formalism can be used to study diblock copolymer melts. The value of χ e N at the critical point of a binary blend exceeds that predicted by Flory-Huggins theory by an amount proportional to 1/√N, though the width of the critical region is proportional to 1/N. For strongly asymmetric blends, however, the binodal value of χ e N is suppressed. The dimensions of individual chains decrease slightly with increasing χ e or with decreasing N, even when χ e = 0. [1] Z.-G. Wang, J. Chem. Phys., 2002, 117:481.

1:51PM V25.00012 Effect of intensity gradient profiles on crystal growth subject to holographic free radical photopolymerization1. THEIN KYU, PANKAJ RATHI, SOOJEOUNG PARK, University of Akron — A theoretical model has been developed to describe a unique phenomenon of photopolymerization-induced crystallization subjected to holographic intensity gradient profiles. A hypothetical phase diagram of a crystalline polymer solution (or blend) is constructed to guide the dynamics of directional crystallization. Calculations of holographic photopolymerization induced crystallization were carried out slightly above the melting temperature of the bends under the conditions of sinusoidal as well as sharp (square) interface. In the case of periodically varying interface, the dynamic calculations revealed that the emerged crystals (spherulites) have out-grown the patterned regions, which is consistent with the crystal growth behavior of the polyethylene oxide/diacrylate system. However, in the case of a sharp holographic the directional growth occurs along the stripes, which is confined within the stratified layers.

1NSF: DMR 0514942.

Thursday, March 13, 2008 11:15AM - 1:03PM –
Session V26 DCP: Focus Session: Advances in Atmospheric Aerosol Science III
Morial Convention Center 218
The vibrational entropic effects stabilize the non-dissociated clusters. This behavior is traced back to the large dynamic effects associated with the formation of nuclei. The free formation energy of the critical cluster plays an essential role in the calculation of nucleation rates. Thus, we have constructed a nucleation rate relation which is easy to calculate and its result is relatively simple to compare with experimental data. The energy formation of a cluster has a few more terms than the traditional classical model. Furthermore, the extra terms in this approach have their roots in the molecular treatment of a cluster formation and they are temperature dependent. We have compared the result of this approach with the original classical theory along with some experimental data. Our initial results seem promising and the temperature correction has a correct trend.

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11:15AM V27.00001 Path Integral Approach to Geometrically Frustrated Quantum Antiferromagnets\textsuperscript{1}, MIRACULOUS BHASEEN, University of Cambridge, JOHN CHALKER, University of Oxford — We develop a path integral approach to geometrically frustrated quantum antiferromagnets. Using Hubbard–Stratonovich transformations to decouple the interactions within clusters of spins, we establish a high temperature expansion of the quantum partition function. This semiclassical approach based on conjugate cluster variables allows us to descend below the Curie–Weiss temperature scale, and to describe the emergent spin liquid regime. We make contact with complementary approaches based on spin wave theory.

\textsuperscript{1}We acknowledge support from EPSRC and the Rudolf Peierls Centre for Theoretical Physics.

11:27AM V27.00002 Contractor-Renormalization approach to frustrated magnets in a magnetic field, ANDREAS ABENDSCHEIN, SYLVAIN CAPPONI, Laboratoire de Physique Théorique, Université Paul Sabatier, CNRS - Toulouse, France — We propose to use the Contractor Renormalization (CORE) technique in order to derive effective models for quantum magnets in a magnetic field. CORE is a powerful non-perturbative technique that can reduce the complexity of a given microscopic model by focusing on the low-energy part. We provide a detailed analysis of frustrated spin ladders which have been widely studied in the past. In particular, we discuss how to choose the building block and emphasize the use of their reduced density matrix. With a good choice of basis, CORE is able to reproduce the existence or not of magnetization plateaux in the whole phase diagram contrary to usual perturbation theory. Furthermore, we present recent results for other, potentially more interesting geometries like the Heisenberg bilayer where we also address the issue of plateau formation and point out the analogy between non-frustrated strongly anisotropic models and frustrated SU(2) ones. Finally, we investigate the magnetization curve of the Shastry-Sutherland model and, however in absence of a magnetic field, we consider the square lattice with four-spin ring-exchange.

11:39AM V27.00003 Spin-orbital liquid state on the square lattice with emergent Majorana fermions and $\mathbb{Z}_2$ topological order, ASHVIN VISHWANATH, FA WANG, UC Berkeley — Magnetism from d-electrons often retains orbital degeneracy which can enhance quantum fluctuations and lead to exotic liquid-like ground states with no conventional order. Indeed, experimental systems like LiNiO$_2$, FeSc$_2$S$_4$ etc. with orbital degeneracy show a lack of order down to low temperatures. We introduce a Majorana-fermion slave particle theory to study such states in spin-1/2 models with $e_g$ orbital degeneracy. This is first applied to a square lattice model with enhanced SU(4) symmetry. A mean field treatment predicts a spin-orbital liquid state with nodal Majorana fermion excitations and $\mathbb{Z}_2$ topological order. A variational Monte-Carlo study of the corresponding wavefunction confirms the absence of magnetic order and bond order, which makes it a candidate state for a spin orbital liquid. Comparing against the exact diagonalization studies in [Bosche et al. Eur. Phys. J. B 17, 367 (2006)], our state is found to have significant overlap with the ground state on small lattices. Despite the absence of a variational parameter, our model can also be tested by finite-size effects and applications to $S=3/2$ atoms confined in optical lattices are pointed out.

11:51AM V27.00004 Magnetic monopoles in spin ices and spin excitations in other pyrochlores\textsuperscript{3}, RODERICH MOESSNER, Max-Planck-Institute for the Physics of Complex Systems — Exotic excitations go along with the unusual ground states of frustrated magnets. One of the most striking examples occurs in dipolar spin ice, where the dipole moment of the underlying electronic spin degrees of freedom fractionalise into magnetic monopoles. This constitutes possibly the first instance of fractionalisation in a three-dimensional material. It enables us to account for a mysterious phase transition observed experimentally in spin ice in a magnetic field, which is a liquid-gas transition of the magnetic monopoles. These monopoles can also be detected by magnetic resonances, e.g., in an experiment modelled after the celebrated Stanford magnetic monopole search. We also discuss other instances of unusual pyrochlore excitations.

\textsuperscript{3}in collaboration with Claudio Castelnovo (Oxford) and Shivaji Sondhi (Princeton)

12:27PM V27.00005 Vortex Berry phases and the magnetization of quantum magnets, AKIHIRO TANAKA, National Institute for Materials Science, KEISUKÉ TOTSUKA, Yokawa Institute of Theoretical Physics, Kyoto University, XIAO HU, National Institute for Materials Science — We revisit the magnetization process of quantum antiferromagnets subject to an external magnetic field, and show how an interpretation in terms of Berry phases emerges. First we develop a continuum variant of the Lieb-Schulz-Mattis- type approach to the 1d problem, and find that the well-known equivalence between solid and liquid behavior is ascribed to the nesting property at the van-Hove singularity preserved under electron correlation. We will also present the results for hyper-Kagome magnets. One of the most striking examples occurs in dipolar spin ice, where the dipole moment of the underlying electronic spin degrees of freedom fractionalises into magnetic monopoles. This constitutes possibly the first instance of fractionalisation in a three-dimensional material. It enables us to account for a mysterious phase transition observed experimentally in spin ice in a magnetic field, which is a liquid-gas transition of the magnetic monopoles. These monopoles can also be detected by magnetic resonances, e.g., in an experiment modelled after the celebrated Stanford magnetic monopole search. We also discuss other instances of unusual pyrochlore excitations.

12:39PM V27.00006 Kinetic ferromagnetism on frustrated lattices, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, KIRILL SHTENGEL, Department of Physics, University of California, Riverside, USA, PETER FULDE, Asia Pacific Center for Theoretical Physics, Pohang, Korea — Systems with frustrated interactions are generally characterized by a high density of low–lying excitations which can be responsible for interesting physical effects. Much attention has been paid to the effects of frustration in antiferromagnetic systems. In this talk, however, we present a model of ferromagnetism arising in a frustrated system. We study strongly correlated electrons described by an extended Hubbard Hamiltonian on a kagome lattice at 1/6 and 1/3 filling. In the limit $t/V \ll 1$, we derive an effective low-energy Hamiltonian for this model. The Perron-Frobenius theorem can then be used to show that the ground state of this system is ferromagnetic. We will address the robustness of ferromagnetism to finite temperature effects and other interactions and discuss possible extensions to other lattices.

12:51PM V27.00007 Magnetic fluctuations in the Hubbard Model on Kagome-based frustrated Lattices, MASAFUMI UDAKAWA, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — We report our results on the interplay between electron correlation and magnetic fluctuations in the geometrically-frustrated Kagome and hyper-Kagome Hubbard models at half filling. These models have two different geometrical units important in the low-energy physics: the frustrated triangle and the non-frustrated loop with even-numbered sites. In order to treat both of them on equal footing, we apply cluster dynamical mean-field theory to large-size clusters up to 12 sites. By calculating the spin susceptibility $\chi(\mathbf{q},\omega)$, we have found in the Kagome system that an anomalous one-dimensional magnetic correlation previously found near the Mott transition [1] is observed even in the non-interacting case at high temperature, and its temperature range gradually suppressed by increasing electron correlation. This behavior is ascribed to the nesting property at the van-Hove singularity preserved under electron correlation. We will also present the results for hyper-Kagome system in relation to the recent experiments on Na$_4$Ir$_2$O$_6$ [2].

1:03PM V27.00008 Study of the $U(1) - Z_4$ cross-over in 2D valence-bond-solids\textsuperscript{1} JIE LOU, ANDERS SANDBVIK, Associate Professor — We consider the 2D Heisenberg model in the overcomplete basis of valence bonds. By tuning matrix elements corresponding closely to the diagonal and off-diagonal terms in Rokhsar-Kivelson quantum dimer model, we show, using a projector quantum Monte Carlo technique, that there is a quantum phase transition into a valence-bond-solid (VBS) state. This system allows us to study the cross-over length-scale \textsuperscript{1}[1] associated with emergent $U(1)$ symmetry of the VBS order parameter \textsuperscript{2}, which has up until now not been possible in other systems \textsuperscript{3}, where the VBS order is weaker and prohibitively large system sizes are needed to observe the stabilization of a manifestly $Z_4$-symmetric VBS. \textsuperscript{[1]} J. Lou, A. W. Sandvik, and L. Balents, Arxiv:0704.1472. \textsuperscript{[2]} T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science 303, 1490 (2004). \textsuperscript{[3]} A. W. Sandvik, Phys. Rev. Lett 98, 227202 (2007).

\textsuperscript{1}Supported by NSF grant DMR-0513930

1:15PM V27.00009 Dimerized Bond-Disordered Quantum Spin Models and Harris Criterion JONAS GUSTAFSSON, Goldman Sachs, DAOXIN YAO,ERICA CARLSON, Purdue University, ANDERS W. SANDBVIK, Boston University — We study several different realizations of dimerized bond disorder in the two-dimensional square-lattice $S=1/2$ Heisenberg model, by introducing strong and weak couplings, $J_s, J_w$, randomly, but in such a way that each spin belongs to one strong bond (a dimer). We study the ground-state phase transition occurring at a critical ratio $g_c = J_s/J_w$ for different ways of distributing the dimers: (a) randomly distributed as in the classical dimer model, whence the dimer-dimer correlation function follows a power law, $c(r) \sim r^{-2}$, and (b) the random plaquette (RP) model, where all dimers are first placed horizontally in columns and thereafter any plaquette with dimers is flipped with probability $p = 1/2$ or 1/4. Our calculations show that the Harris criterion for the relevance of disorder is not applicable to these models. In all cases, the disorder does not appear to change the universality class from that obtaining with a regular dimer arrangement.

1:27PM V27.00010 Spontaneous parity breaking of Dirac spin liquid in a magnetic field, YING RAN, University of California, Berkeley, WING-HO KO, PATRICK LEE, XIAO-GANG WEN — The Dirac spin liquid was proposed to be the ground state of the spin-1/2 Kagome antiferromagnets. In a magnetic field, we show that the state with Fermi pocket is unstable to the Landau level (LL) state and the XY ordered state. We mainly focus on the fully gapped LL state, which breaks parity symmetry and thus supports a finite temperature phase transition. We discuss experimental signatures which we can be focus on the fully gapped LL state, which breaks parity symmetry and thus supports a finite temperature phase transition. We discuss experimental signatures which we can be

1:39PM V27.00011 Two-step spin flop transition in quantum spin ladders, TORU SAKAI, Japan Atomic Energy Agency and CREST JST, KYIOMI OKAMOTO, Tokyo Institute of Technology — It is well known that the antiferromagnet with easy-axis anisotropies exhibits a field-induced first-order phase transition, the so-called spin flop. In one-dimensional quantum spin systems, instead of it, a second-order phase transition occurs because of large quantum fluctuations\textsuperscript{1}. Particularly the $S=1$ antiferromagnetic chain with the easy-axis single-ion anisotropy was revealed to exhibit two successive field-induced second-order transitions by our previous numerical analysis\textsuperscript{2}. However, such transitions have not been observed yet. Recently a two-step spin flop transition was observed in the spin ladder system IPA-CuCl$_4$\textsuperscript{3}, which has ferromagnetic rung coupling. In order to clarify the mechanism of the two-step field-induced transition, we investigate the anisotropic spin ladder using the numerical diagonalization and the finite-size scaling analysis. As a result, we revealed that two different field-induced second-order quantum phase transitions possibly occur. Several phase diagrams are also presented. In addition we discuss on a possible two-step spin flop in other materials\textsuperscript{4} and some frustrated systems. \textsuperscript{[1]} C. N. Yang and C. P. Yang, Phys. Rev. 151 (1966) 258. \textsuperscript{[2]} T. Sakai, Phys. Rev. B 58 (1998) 6268. \textsuperscript{[3]} T. Masuda et al, Phys. Rev. Lett. 96 (2006) 047210. \textsuperscript{[4]} H. Miyasaka et al, Inorg. Chem. 42 (2003) 8203.

1:51PM V27.00012 Spin and Singlet Dynamics of the S=1/2 Quantum Kagome Antiferromagnet, ANDREAS LAUCHLI, IRMMA — EPF Lausanne, Switzerland, CLAIRE LHUILLIER, LPTMC, UPMC Paris, France — The Kagome Heisenberg antiferromagnet with spin 1/2 has been the topic of many theoretical investigations. Most of these focused on groundstate properties or were aiming at an explanation of the anomalous high density of singlet excitations. In this contribution we report on exact diagonalization studies concentrating on dynamical correlation functions. First the full dynamical spin structure factor $S(q, \omega)$ on 36 sites has been obtained, showing a broad, rather incoherent spectral response, which furthermore seems to increase significantly at low energies. Then we discuss the time dependent spin autocorrelation function as well as dynamical dimer-dimer correlation functions. All these results combined point towards a highly fluctuating system, both in the singlet and the triplet channel. We conclude by a comparison with recent inelastic neutron scattering measurements on the Herbertsmithite and Volborthite compounds.

2:03PM V27.00013 Pseudo-Dirac Hamiltonians and Flux Phases of SU(N) magnets, F.J. BURNELL, S.L. SONDHI, Princeton University, R. SHANKAR, Yale University — The lattice Dirac Hamiltonian describes a particle hopping on a lattice in a particular background magnetic field. We present a family of hopping Hamiltonians in other background fields that generalize many aspects of the Dirac Hamiltonian to lines and planes of nodes. In our canonical case, hopping on the pyrochlore lattice gives rise to a half filled fermi surface that consists of four intersecting \cite{111} lines. This spectrum is invariant under tetrahedral rotations, rather than all rotations as in the Dirac case, resulting in a more complex matrix anti-commutation structure. This structure arises in a large N treatment of the SU(N) Heisenberg model on the pyrochlore.


11:51 AM V28.00002 Backward-wave optical parametric amplification and mirrorless oscillations in negative-index materials

T. F. George and V. M. Shalaev, Purdue University — Extraordinary properties of mirrorless backward-wave OPO in nanostructured crystal have been recently demonstrated in [1]. Phase matching of backward waves is inherent to negative-index materials (NIMs). Extraordinary, distributed-feedback, properties of OPA and possibility of OPO in NIMs were predicted in [2,3]. Herewith, we show the feasibilities and explore the features of the mirrorless OPO and of the generation of counterpropagating left-handed signal and right-handed idler photons in NIMs. Two different options are investigated. One is OPO based on intrinsic quadratic nonlinearity of the NIM. Another option is four-wave mixing OPO based on separately engineered strong cubic nonlinearity through resonant nonlinear impurities. It is shown that in the latter case the OPO properties can be tailored by quantum control.

Support by the ARO W911NF-0710261 and ARO MURI 50342-PH-MUR awards.

12:03PM V28.00003 Tunable photonic crystals with nonlinear composite materials

KIN WAH YU, Chinese University of Hong Kong, Shatin, NT, Hong Kong. J. P. HUANG, G. WANG, Fudan University, Shanghai, China — Photonic crystals (PCs) are periodic dielectric structures that are designed to control the flow of electromagnetic (EM) waves. The main attraction of PCs is the existence of photonic band gaps, for frequencies within which the propagation of EM waves can be forbidden leading to many promising applications in the areas of computing and communication for their advantages over electronics. In this work, we report a novel class of tunable photonic crystals consisting of multilayers of noble-metal nanoparticles in dielectric composites with nonlinear responses [1]. For such PCs, precise tunability of photonic band gaps can be achieved by choosing appropriate pump AC or DC electric fields [2]. Moreover, we study the dynamics of Bloch oscillation in such PCs so as to realize terahertz radiation which is relevant in medical physics.


Supported by RGC Earmarked Grant of Hong Kong SAR Government.

12:15PM V28.00004 Enhanced and Resonant Transmission of Light through Dielectric-filled Subwavelength Waveguides

HUIZHONG XU, PANGSHUN ZHU, HAROLD G. CRAIGHEAD, WATT W. WEBB, School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853 — We analyze transmission of light through dielectric-filled subwavelength waveguides in a metal using both analytical and numerical methods. Our analysis revealed that a propagating mode can in principle exist in a waveguide of arbitrarily small size when a certain relationship between the dielectric constants of the metallic cladding and filling material is satisfied. Transmission through a subwavelength aperture of finite length can be further enhanced when the length is such that Fabry-Pérot-like resonances are excited. Strong, localized near-field intensity at the exit can be achieved with this mechanism for aperture diameters down to ~\(\lambda/20\). We will describe potential applications of this resonantly enhanced transmission phenomenon in near-field scanning optical microscopy and single-molecule spectroscopy.

This research is supported by NIH grant No. 9-P41-EB001976, NSF grant No. DMR-0520404, and the STC program of the NSF under agreement No. ECS-9876771.

12:27PM V28.00005 Transmission of images with subwavelength resolution to distances of several wavelengths in microwave, terahertz and infrared ranges

PAUL BELOV, Queen Mary University of London, UK, MARIO SILVEIRINHA, University of Coimbra, Portugal, PEKKA IKONEN, CONSTANTIN SIMOVSKI, SERGEI TRETYAKOV, Helsinki University of Technology, FINLAND, YAN ZHAO, YANG HAO, CLIVE PARINI, Queen Mary University of London, UK — The resolution of conventional imaging systems is restricted by the diffraction limit: the details smaller than half-wavelength of radiation cannot be resolved. Using novel engineered media with extreme optical anisotropy and waveguiding properties it is possible to overcome the classical limit and create devices capable of transmitting images with subwavelength resolution over long distances. We report experimental results that demonstrate transmission of a microwave image by means of an array of parallel metallic rods over a distance 3.5 times greater than the wavelength. The resolution of such imaging device is 15 times less than the wavelength. The magnifying, demagnifying and repeating properties of lenses formed by long metallic rods provide a unique solution for subwavelength imaging at microwave and terahertz ranges. At microwave wavelengths, the resolution of such lenses is mainly determined by the characteristic period, which is limited only by the fabrication capability rather than by any physical constraints. At higher frequencies, the resolution is mainly limited by the skin-depth of the rods material.

This research was sponsored through NSF-NIRT grant No. 0304678.

12:39PM V28.00006 All Optical Method for Positioning Single Quantum Dots in Photonic Crystal Nanocavities

SUSSANNA THON, MATTHEW RAKHER, JAN GUDAT, HYOCHUL KIM, WILLIAM IRVINE, DIRK BOUWMEESTER, University of California Santa Barbara, Department of Physics, NICK STOLTZ, PIERRE PETROFF, University of California Santa Barbara, Materials Department — Single self-assembled InAs quantum dots embedded in GaAs photonic crystal (PC) defect cavities are a promising system for cavity quantum electrodynamics experiments. Achieving controllable coupling between the PC cavity mode and quantum dot emission is difficult, however, due to the random nucleation locations and spectral properties of individual quantum dots. We have developed a novel, all optical scheme for locating single dots relative to prefabricated markers on the sample surface with sub-10 nm accuracy which should allow us to custom fabricate PC cavities tuned to the exact position and frequency of the quantum dots. Initial experimental results are presented.

This research was sponsored through NSF-NIRT grant No. 0304678.

12:51PM V28.00007 Effect of Shape Parameters on NanoOptronic Circuit Element Optical Response

TIMOTHY CORRIGAN, University of Maryland, Department of Physics, College Park, MD and University of Maryland, Materials Science, College Park, MD, DOMINIC BRITTI, University of Maryland, Materials Science, College Park, MD, PAUL KOLB, Laboratory for Physical Sciences, College Park, MD, ANDRIE SUSHKOV, DENNIS DREW, University of Maryland, Department of Physics, College Park, MD, SHYHUAH GUO, University of Maryland, Electric Engineering, College Park, MD and Laboratory for Physical Sciences, College Park, MD, RAYMOND PHANEUF, University of Maryland, Materials Science, Physics, and Electric Engineering, College Park, MD, and Lab for Physical Sciences, College Park, MD — We examine the effect on the visible-near IR response of a number geometrical parameters of optical circuit elements with potential applications for guiding light for communications and for use in other metamaterial/optoelectronics applications. Rounding of edges produces a shift in the resonance frequency transmission measurements and in numerical simulations. We also examine the effect of shape parameters on the response of u-shaped and single split-ring Ag structures and discuss the LC circuit model in describing their optical response.

Work supported by the Lab for Physical Sciences.
non-contact method for patterning three-dimensional carbon nanotube microstructures. In this method, a 1 \mu m, WEI-HUSUAN HUNG, RAJAY KUMAR, ADAM BUSHMAKER, MICHAEL J. BRONIKOWSKI, STEPHEN B. CRONIN — We present an optical, measurements of such nanodevices is our future goal.

In particular, it was possible to drill 2.5 nm diameter nanoholes in multiwall carbon nanotubes (MWNT’s). Similarly sized holes were etched through metallic nanowires. We have also fabricated larger nanoholes, as large as 11 nm wide in a 26 nm diameter MWNT, as well as constrictions in MWNT’s. Transport has unusual and potentially useful electrical transport properties. Local control of the parameters of such nano-objects would open even wider possibilities for their applications. We have used the highly focused, high-energy electron beam of a transmission electron microscope to locally modify such nano-objects.

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THOMAS AREF, UIUC, MIKAS REMEIKA, UCSD, MATTHEW BRENNER, ALEXEY BEZRYADIN, UIUC — Carbon nanotubes and metallic nanowires have unusual and potentially useful electrical transport properties. Local control of the parameters of such nano-objects would open even wider possibilities for their applications. We have used the highly focused, high-energy electron beam of a transmission electron microscope to locally modify such nano-objects. In particular, it was possible to drill 2.5 nm diameter nanoholes in multiwall carbon nanotubes (MWNT’s). Similarly sized holes were etched through metallic nanowires. We have also fabricated larger nanoholes, as large as 11 nm wide in a 26 nm diameter MWNT, as well as constrictions in MWNT’s. Transport measurements of such nanodevices is our future goal.

11:15AM V29.00001 High-Resolution Nanofabrication Using a Highly-Focused Electron Beam, THOMAS AREF, UIUC, MIKAS REMEIKA, UCSD, MATTHEW BRENNER, ALEXEY BEZRYADIN, UIUC — Carbon nanotubes and metallic nanowires have unusual and potentially useful electrical transport properties. Local control of the parameters of such nano-objects would open even wider possibilities for their applications. We have used the highly focused, high-energy electron beam of a transmission electron microscope to locally modify such nano-objects. In particular, it was possible to drill 2.5 nm diameter nanoholes in multiwall carbon nanotubes (MWNT’s). Similarly sized holes were etched through metallic nanowires. We have also fabricated larger nanoholes, as large as 11 nm wide in a 26 nm diameter MWNT, as well as constrictions in MWNT’s. Transport measurements of such nanodevices is our future goal.

11:27PM V28.00010 Wavefront Analysis as a Predictive Tool for Polymer/Liquid Crystal Composites with Nanostructures, JARED COYLE, SAMEET SHRIYAN, ADAM FONTECCHIO, Drexel University — Nano-scale morphology is a key factor in determining the optical performance of holographically-formed polymer dispersed liquid crystal (HPDLC) thin films. The liquid crystal(LC)/polymer interface and droplet structure in these materials effects optical performance. Established microscopy techniques such as SEM and TEM are conventionally used to examine interfacial properties. In this paper, HPDLC reflective and transmissive wavefront analysis are used to examine gratings created using three different polymer formulations: acylate, thiol-ene and a combination of acylate and thiol-ene. Changes in the modulation transfer function, Strehl ratio and wavefront phase of both transmissive and reflective wavefronts are compared to morphological properties shown in SEM images. Wavefront properties were measured using a Shack Hartman wavefront analyzer. Optical performance characteristics were measured using an Ocean Optics spectrometer, halogen light source and oscilloscope.


11:27AM V29.00002 Optical Patterning of Three-Dimensional Carbon Nanotube Microstructures, WEI-HUSUAN HUNG, RAJAY KUMAR, ADAM BUSHMAKER, MICHAEL J. BRONIKOWSKI, STEPHEN B. CRONIN — We present an optical, non-contact method for patterning three-dimensional carbon nanotube microstructures. In this method, a 1 \mu m diameter focused laser spot is used to burn patterns in dense arrays of vertically grown multiwalled carbon nanotubes. The threshold for laser burnout and the depth of burnout are determined by Raman spectroscopy and scanning electron microscopy. Using a high precision translation stage to control the position of the laser spot on the sample, we create several 3D patterns to illustrate this method’s potential use for the rapid prototyping of carbon nanotube microstructures [1]. After laser surface treatment, we observe undercut profiles, changes in nanotube density, and nanoparticle formation, which provide insight into the unique evolution of the nanotube microstructures during the burnout process. This non-lithographic method provides new opportunities for chemically sensitive applications of nanotubes and expands their possible applications into new areas.


11:39AM V29.00003 A Real Time Detection System for Dielectrophoretic Deposition of Carbon Nanotubes, SEBASTIAN SORGENFREI, INANC MERIC, AUSTIN AKYE, SARBAJIT BANERJEE, SAMI ROSENBLATT, IRVING P. HERMAN, KENNETH SHEPARD, Columbia University — Single-walled carbon nanotubes (SWCNTs) have showed considerable potential as building blocks for electronics and sensors but are very difficult to integrate and assemble into larger systems. Dielectrophoretic deposition allows the large-scale positioning and alignment of SWCNT’s but requires precise control to reproducibly generate single-tube devices. We investigate dielectrophoretic deposition of SWCNT’s using an in situ detection system. This apparatus locks into both a small AC signal and the large, mixed-down dielectrophoretic signal, generated by the nonlinearities of the device, making it possible to halt deposition once a nanotube has made electrical contact. This results in a higher yield of single SWCNT’s deposited between two electrodes.

This work was supported in part by the SRC Focus Center Research Program through the C2S2 Center and by the NSF under Grant 0707748.
11:51AM V29.00004 Irradiation-induced phenomena in carbon nanomaterials  ARIKDY KRASHENIN-NIKOV, Accelerator Laboratory, University of Helsinki, and Laboratory of Physics, Helsinki University of Technology, Finland — The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments [for an overview, see A.V Krasheninnikov, F. Banhart, Nature Materials, 6 (2007) 723] on bombardment of carbon nanostructures with energetic particles demonstrate that irradiation can have beneficial effects and that electron or ion beams may serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of nanostructured carbon systems. We systematically study irradiation effects in carbon nanotubes and other forms of nano-structured carbon experimentally and theoretically by employing various atomistic models ranging from empirical potentials to time-dependent density functional theory. In my presentation, I will briefly review the recent progress in our understanding of ion-irradiation-induced phenomena in nano-structured carbon and present our recent theoretical [A.V Krasheninnikov, et al., Phys. Rev. Lett., 99 (2007) 016104, A. Tolvanen et al., Appl. Phys. Lett. 91 (2007) 173109.] and experimental [O. Lehtinen et al., to be published] results. I dwell on the “beneficial” role of defects and impurities in nanotubes and related systems. Finally, I will present the results of simulations of irradiation-induced pressure build-up inside nanotubes encapsulated with metals [L. Sun, et al., Science 312 (2006) 1199]. Electron irradiation of such composite systems in the transmission electron microscope gives rise to contraction of nanotube shells and thus to high pressure. The irradiation-stimulated pressure can be as high as 40 GPa, which makes it possible to study phase transformations at the nanoscale with high spatial resolution. I will also address the mechanisms of plastic deformation of small metal particles inside carbon shells at high temperatures, which may be important for understanding catalytic growth of carbon nanotubes.

12:27PM V29.00005 Syntheses and characterization of SWCNT assemblies prepared on silicon substrates with different methods of patterning catalyst particles  IRMA KULJANISHVILI, VENKAT CHANDRASEKHAR, Department of Physics and Astronomy, Northwestern University, OWEN LOH, DMITRIY DIKIN, HORACIO ESPINOSA, Department of Mechanical Engineering, Northwestern University, RICHARD PINER, RODNEY S. RUOFF, Department of Mechanical Engineering, University of Texas at Austin — Techniques for controlled way of preparation of single wall carbon nanotubes (SWCNT) on substrates continue to be of interest, including for potential applications in integrated circuits and nanodevices. We report on our work, undertaken to elucidate a number of favorable conditions for controlled patterning and growth of high quality SWCNT. Synthesis is carried out under ambient pressure with methane used as feed gas. A key factor for successful SWCNT growth is known to be the catalytic precursor. We compare several methods of controlled deposition of the catalyst precursors on oxidized silicon substrates using methods such as e-beam lithography, photolithography and screening probe writing methods that allow for maximum flexibility and high efficiency for incorporating SWCNTs into devices or circuit architectures. The advantages and some limitations of these methods of selective patterning will also be addressed. Analysis and characterization of the as-grown SWCNTs was performed by Raman Spectroscopy, AFM and SEM.

12:39PM V29.00006 In-situ calorimetric studies of SWCNT growth  OLEG KUZNETSOV, TOSHIO TOKUNE, ELENA MORA, GUGANG CHEN, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc. — Single-walled carbon nanotubes (SWCNTs) were grown inside of a differential scanning calorimeter (DSC) apparatus with an attached mass spectrometer (MS), using different hydrocarbons (CH₄ and C2H₆) and alumina supported (Fe, Fe/Mo, and Ni) catalysts. This set-up allowed to in situ follow the evolution of calorimetric, thermogravimetric and MS data during the synthesis. A Raman spectrometer (with laser excitations wavelengths 532 and 785 nm) was used for verification of the growth of SWCNTs. DSC studies at temperatures ∼650-900 °C of the interaction between the hydrocarbons and the preliminary reduced alumina supported catalysts showed a release (C2H2) or absorption (CH4) of heat depending on the type of hydrocarbon used. The effect of this energy on the growth of SWCNTs was studied. We found that the incubation time for nanotube nucleation depends on the hydrocarbon type and flow rate, as well as on the synthesis temperature. The origin of the initial endothermic peak observed during nanotube growth with both hydrocarbon sources will be discussed. Furthermore, the kinetics and thermodynamic of hydrocarbon decomposition, carbon atoms diffusion and solid carbon structure formation dependence on the catalyst and synthesis parameters will also be presented.

12:51PM V29.00007 The role of carbon solubility in Fe-C nano-clusters on the growth of small single-walled carbon nanotubes  STEFANO CURTAROLO, NEHA AWASTHY, WAHYU SETYAWAN, Duke University, ELENA MORA, TOSHIO TOKUNE, Honda R.I., KIM BOLTON, Göteborg University, AVETIK HARUTYUNYAN, Honda R.I. — Various diameters of alumina-supported Fe catalysts are used to grow single-walled carbon nanotubes (SWCNTs) with chemical vapor decomposition. We find that the reduction of the catalyst size requires the incubation time for nanotube nucleation on the hydrocarbon type and flow rate, as well as on the synthesis temperature. The origin of the initial endothermic peak observed during nanotube growth with both hydrocarbon sources will be discussed. Furthermore, the kinetics and thermodynamic of hydrocarbon decomposition, carbon atoms diffusion and solid carbon structure formation dependence on the catalyst and synthesis parameters will also be presented.

1:03PM V29.00008 Air assisted growth of long aligned carbon nanotube films  XIANFENG ZHANG, RAKESH SHAH, SAIKAT TALATAPRA, Department of Physics, Southern Illinois University Carbondale — We report on air assisted growth of ultra long aligned bundles of multiwall carbon nanotubes. We found that the growth rate of carbon nanotubes is highly enhanced by introducing a small amount of oxygen during the catalytic decomposition of ferrocene-xylene mixture at 750°C. Millimeter long aligned carbon nanotube films were easily synthesized on silicon dioxide as well as metal substrates by controlling the air flow. Electron microscopy investigations reveal that the films are composed of dense aligned multi-wall CNTs with the diameters ranging from about 30-100 nm. We will also present our preliminary results on the electrical transport measurement performed on these long nanotube bundles.

1:15PM V29.00009 Boron-Doped Carbon Nanotube Films  XIAO MING LIU, H.E. ROMERO, H.R. GUTIERREZ, P.C. EKLUND — Here we report room temperature optical and resistivity studies on transparent thin films of bundled single-walled carbon nanotubes exposed to B₂O₃ at 1000°C. This reaction is proposed to B-dope the films. They are stable in air. At 300K the four-probe sheet resistance and the optical transmission in the NIR-UV range are used to evaluate the effects of this chemical exposure. Our preliminary results show that for films with a visible optical transmittance around 80% (550nm), the sheet resistance in the pristine film is lowered from ~2KΩ to ~300Ω via B₂O₃ exposure, a factor of five decrease. We find that the magnitude of the decrease in the sheet resistance increases in samples with higher transmission. Our results suggest that boron-doped SWNT may provide a better approach to touch-screen technology, as well as for transparent contacts in solar cells.
The atomistic approach combines Monte Carlo methods with total energy electronic structure methods to explore island formation, growth, and lift-off dynamics. This method allows for the simulation of the growth process and provides insights into the energetics of the growth steps. Transient interruptions or changes in hydrocarbon flow are revealed by rapid changes in slope and frequency of the oscillating, exponentially-decaying TRR signal. The associated regions of the nanotube array reveal kinked, band-like patterns along the width of the array as observed in cross-sectional scanning electron microscopy (SEM) images. These bands serve as ‘growth-markers’ to measure length intervals and calibrate growth rates before, during, and after transient perturbations to continuous growth. In addition, extended growth interruptions are explored to understand catalyst poisoning mechanisms. Finally, growth of size-selected, multilayered VANTAs was performed to investigate the interfaces between different growth regions by HRTEM.

1:39PM V29.00011 Chirality-resolved kinetic analysis of single-walled carbon nanotube growth by in-situ Raman spectroscopy, TAKASHI UCHIDA, MASAYA TAZAWA, HIROSHI SAKAI, AKIRA YAMAZAKI, YOSHIHIRO KOBAYASHI, NTT BASIC RESEARCH LABORATORIES TEAM, CREST/JST TEAM, TOKYO UNIVERSITY OF SCIENCE COLLABORATION, MEJII UNIVERSITY COLLABORATION — We investigate the chirality-resolved growth kinetics of single-walled carbon nanotubes (SWCNTs) by in-situ Raman spectroscopy. The SWCNTs are synthesized by ethanol CVD from Co nanoparticle catalysts with pre-defined size before the CVD process. The chirality-sensitive radial breathing mode (RBM) signals in Raman spectra are observed during the CVD process at 80-120 Pa. We have reasonably assigned the chiral indices of the RBM signals observed at higher temperature during the CVD process by taking into account the temperature dependence of the resonance condition of SWCNTs. The growth kinetics analysis from the time evolution of each RBM signal in in-situ spectra reveals that the nanotube nucleation occurs just after the supply of the carbon source gas and does not significantly depend on the growth pressure and chirality. In addition, we have found that the growth duration depends on the growth pressure and chirality and that the graphitic encapsulation of catalyst particles terminates SWCNT growth. These findings make it possible to clarify the chirality-sensitive growth behavior of SWCNTs.

2:03PM V29.00013 Understanding the Growth of Carbon Nanotubes by Catalyst-Assisted Chemical Vapor Deposition, ELIF ERTEKIN, UC Berkeley, JEFFREY GROSSMAN, COMPUTATIONAL NANOSCIENCE GROUP TEAM — In catalyst-assisted chemical vapor deposition, carbon nanotubes are formed when a curved graphene island lifts off the surface of the catalyst particle on which it is growing. While this growth technique offers effective control over patterning and alignment, control over nanotube radius and chirality is ultimately tied to understanding the point at which lift-off occurs. We use atomistic approaches to model the lift-off process via the interplay between the excess energy required to grow a curved (and thus, necessarily defected) graphene island and the interaction energy between the growing island and the underlying catalyst. The monodomain approach combines Monte Carlo and molecular dynamics methods to study the formation, growth, and lift-off of nanotubes on a catalyst surface. Using this approach, we are able to systematically study the effect of incident atomic flux rate, growth temperature, and catalyst curvature. The different defect topologies in the growing graphene cap that result from different growth conditions are a key parameter in determining the chirality of the nanotubes.
Torsion-induced conductance oscillations have been recently observed in multi-wall nanotube \(\delta \phi\) subbands allowed in the nanotube, whereas a change in registry should give rise to a simple inverse dependence. \(\delta \phi\) is the Fermi level shift across subbands vs \(1/d^2\). Hence, the experimental results validate the interpretation of Fermi level shift across subbands related to registry change, as a source of torsion-induced conductance oscillations in carbon nanotubes.

\[\delta \phi \sim \frac{1}{d^2}\]

This dependence is theoretically predicted from the shifting of the corners of the first Brillouin zone of graphene across different subbands allowed in the nanotube, whereas a change in registry should give rise to a simple inverse dependence. \(\delta \phi \sim 1/d^2\). Hence, the experimental results validate the interpretation of Fermi level shift across subbands related to registry change, as a source of torsion-induced conductance oscillations in carbon nanotubes.

\[\delta \phi \sim \frac{1}{d^2}\]

Not only does the precision, low cost, reproducibility and parallelism of our new process create novel opportunities for the implementation and investigation of complex nanosystems, but it also enables us to gain insight into the dynamics of molecular interactions between nanoscale objects of mega-daltons size.

1Equal contribution
2Equal contribution
3Equal contribution

11:51AM V30.00004 Diameter-dependent conductance oscillations in carbon nanotubes upon torsion. NAGAPRIYA K.S., Weizmann Institute of Science, Rehovot, Israel. TZAHI COHEN-KARNI, LIOR SEGEV, ONIT SRUR-LAVI, SIDNEY COHEN, ERNESTO JOSELEVICH, Weizmann Institute of Science, Rehovot, Israel. — Torsion-induced conductance oscillations have been recently observed in multi-wall carbon nanotubes. These oscillations have been interpreted as metallic-semiconductor periodic transitions, while an alternative interpretation attributed the phenomenon to changes in registry between the walls. Here we show that the period of the oscillations is inversely proportional to the squared diameter of the nanotube \(\sim \frac{1}{d^2}\). This dependence is theoretically predicted from the shifting of the corners of the first Brillouin zone of graphene across different subbands allowed in the nanotube, whereas a change in registry should give rise to a simple inverse dependence \(\sim \frac{1}{d^2}\). Hence, the experimental results validate the interpretation of Fermi level shift across subbands related to registry change, as a source of torsion-induced conductance oscillations in carbon nanotubes.


12:03PM V30.00005 Nanomechanical properties of carbon nanotubes determined using a scanning laser vibrometer. LAURA BIEDERMANN, RYAN TUNG, ARVIND RAMAN, RONALD REIFENBERGER, Birck Nanotechnology Center, Purdue University. — To better understand the nanomechanical properties of nanotubes and nanowires, reliable nondestructive techniques that measure their Young’s modulus, \(E\), under ambient conditions are needed. Using a scanning laser vibrometer, the thermally excited eigenfrequencies of plasma-enhanced carbon vapor deposition (PECVD) multiwalled carbon nanotubes (MWNTs) were measured. Due to the small diameters involved, little light is reflected from a bare MWNT. By carefully attaching a small Au-coated glass bead, the intensity of reflected light is sufficiently increased to allow accurate measurements. The length and diameters of the MWNTs are determined using electron microscopy, allowing \(E\) to be inferred from an Euler-Bernoulli analysis of a pinned cantilever beam. A unique aspect of our work is that the attached glass bead exerts a torque on the MWNT. A resonance, attributed to a torsional oscillation, appears for the laden MWNTs, allowing an estimate for the torsional modulus \(G\). Values measured for \(E\) and \(G\), along with a description of the experimental procedure, will be presented at the talk.

12:15PM V30.00006 Mechanical Sensing with Flexible Metallic Nanowires. VLADIMIR DOBROKHOTOV, MEHDI YAZDANPAZH, SANTOSH PABBA, ABDULLAH SAFIR, ROBERT COHN, ElectroOptics Research Institute and Nanotechnology Center University of Louisville. — A calibrated method of force sensing is demonstrated in which the buckled shape of a long flexible metallic nanowire is interpreted to determine the applied force. Using a nanomanipulator the nanowire is buckled in the chamber of a scanning electron microscope (SEM) and the buckled shapes are recorded in SEM images. Force is determined as a function of deflection for an assumed elastic modulus by fitting the shapes using the generalized elastica model. In this calibration the elastic modulus was determined using an auxiliary AFM measurement, with the needle in the same orientation as in the SEM. Following this calibration the needle was used as a sensor in a different orientation than the AFM coordinates to detect a suspended PLLA polymer fiber from which the elastic modulus (2.96 GPa) was determined. In this study the same needle remained rigidly secured to the AFM cantilever beam throughout the entire SEM/AFM calibration procedure and the characterization of the nanofiber.

12:27PM V30.00007 c-axis GaN nanowires for high-quality-factor mechanical oscillators. JASON GRAY, University of Colorado, KRIS BERTNESS, NORMAN SANFORD, National Institute of Standards and Technology, CHARLES ROGERS, University of Colorado. — We report on the electromechanical properties of c-axis GaN nanowires in high-quality-factor mechanical resonators and oscillators. The nanowires are grown by catalyst-free molecular beam epitaxy, are single crystal, hexagonal in cross section, from 50 - 500 nm diameter, and 5 - 15 microns in length depending upon growth time. As-grown nanowires display singly-clamped cantilever mechanical resonances above 1 MHz, with typical resonance full width at half maximum power of less than 100 Hz i.e., a mechanical quality factor, \(Q\), well above 10^4. We are attempting to obtain similar high-\(Q\) for processed nanowires, utilizing dielectrophoresis to position the nanowires within lithographic test structures, and nanowire metallization of two types: First, titanium/aluminum over the ends of the nanowires allows for ohmic contact formation and direct measurement of nanowire resistance versus strain. Second, a layer of aluminum over the entire length of the wires leads to a metallic backbone with a resistance on the order of 50 \(\Omega\). This is useful for simple magnetomotive measurements. We will discuss the processing steps and observed behavior.

With support from GE and the Interdisciplinary Micro/Nano Electromechanical Transducers Center (iMINT) at CU-Boulder.

12:39PM V30.00008 Self-detecting mechanical resonators made from suspended carbon nanotubes. BENITO WITKAMP, MENNO POOT, ANDREAS K. HÜTTTEL, HERRE S.J. VAN DER ZANT, Delft University of Technology. — We study the flexural and torsional mechanical properties of suspended carbon nanotubes. We have used a suspended carbon nanotube as a frequency mixer to detect its own mechanical motion. A single gate-dependent resonance is observed, which we attribute to the fundamental bending mode vibration of the suspended carbon nanotube. Using a continuum model fit to the measurements, we show that the nanotubes in our devices have no slack and that, by applying a gate voltage, the nanotube can be tuned from a regime without strain to a regime where it behaves as a vibrating string under tension. We are currently investigating the low-temperature properties of these devices. We are also investigating the torsional mechanical properties of nanotubes.
12:51PM V30.00009 Characterization and wear resistance of carbon nanotube-based tips for AFM local anodic oxidation nanolithography, LISHAN WENG, Department of Physics, Purdue University, MARK STRUS, ARVIND RAMAN, Department of Mechanical Engineering, Purdue University, LEONID ROKHINSON, Department of Physics, Purdue University — The AFM local anodic oxidation (LAO) lithography is a powerful scanning-probe-based patterning technique for fabrication and post-fabrication tuning of nanoscale structures and devices. The conventional tips suffer from rapid wear which degrades the quality of imaging and LAO lithography. Much research has been devoted to seek for wear-resistant AFM tips, and carbon nanotubes (CNT) are viable candidates. Apart from featuring small diameter, high aspect ratio, and mechanical flexibility, the CNT tips have been shown to last longer during LAO. We investigate the wear of CNT-based tips during LAO lithography by imaging the tips before and after the lithography using scanning electron microscope. CNTs show small contamination on the tip apex while preserve their original length and diameter after more than 200 micron of the lithography. We also analyze tip-surface interaction in order to optimize the quality of lithography and correlate energy dissipation during tapping mode to the line width and line thickness during LAO.


1:15PM V30.00011 Cavity-controlled, electrically-induced infrared emission from a single-wall carbon nanotube, FENGXIAO XIA, MATHIAS STEINER, YU-MING LIN, PHAEDON AVOURIS, IBM Watson Research Center — Single-wall carbon nanotube (SWCNT) is attracting significant attention from the photonics community recently due to its unique optical properties and potential applications in optical communications, optical interconnects, and, in particular, nanophotonics. Tunable and truly nanometer-scale (diameters of 0.5 to 2nm) light emitters can possibly be realized using individual semiconducting nanotubes. However, optical cavities are needed to control the emission wavelength, direction, and emission rate of these broadband, nanoscale emitters. Here, we report the monolithic integration of an electrically-excited light emitter based on a single (SWCNT) with a planar photonic λ/2-cavity. Emission properties were dominated by the cavity characteristics almost regardless of the free-space emission. The broad, free-space emission spectrum of a single SWCNT with a FWHM of 300 to 500nm was transformed to cavity controlled emission with a FWHM of ~40nm. We also modeled the device as a broadband emitter in a planar cavity. Good agreement between the simulated and experimental results was achieved. In our configuration, the maximum enhancement in emission rate is estimated to be 4.4. We consider this result to be an important first step in the development of truly nanometer-scale photonic devices based on SWCNTs.

1:27PM V30.00012 Fluorination and Defluorination of Double-wall Carbon Nanotubes, JUNCHO KANG, MERYL PULIKATHARA, VALERY KHABASHESKU, KEVIN KELLY, RICE University — Due to the unique physical structure double-wall carbon nanotubes (DWNTs), the outer tube can be chemically functionalized while the inner tube is left in pristine condition. Using a fluorinating agent, DWNTs are fluorinated and X-ray photoelectron spectroscopy data indicates that the resulting product composition is equivalent to C3F. The diameter of bare DWNTs is around 2-3 nm as measured by scanning tunneling microscopy, but fluorinated DWNTs possess much larger diameters in a range from 3-10 nm due to a stronger electronic interaction. In addition to imaging the as prepared material, the material was imaged after annealing at temperatures up to 650 K. Due to defluorination, the diameter is decreased down to that of the initial bare DWNTs and atomic resolution of the lattice was recovered. In addition, it was possible to observe that the initial and final structures on the same nanotubes and the evolution of their associated defect structures. Lastly, Raman spectroscopy was employed to confirm the defluorization by revealing the recovery of the RBM peak which disappeared upon fluorination.

1:39PM V30.00013 Magnetic studies of multi-walled carbon nanotube mats: Ultra-high temperature ferromagnetism or superconductivity?, PIETER BEELI, GUO-MENG ZHAO, Department of Physics and Astronomy, California State University, Los Angeles — We report magnetic measurements up to 1200 K on multi-walled carbon nanotube mats using a Quantum Design vibrating sample magnetometer. Extensive magnetic data consistently show two ferromagnetic-like transitions at about 1000 K and 1275 K, respectively. The lower transition at about 1000 K is associated with an Fe impurity and its saturation magnetization is in quantitative agreement with the Fe concentration measured with a vibrating sample magnetometer. Extensive magnetic data consistently show two ferromagnetic-like transitions at about 1000 K and 1275 K, respectively. The lower transition at about 1275 K is consistent with ferromagnetism of any carbon-based phases or magnetic impurities but with the paramagnetic Meissner effect due to the existence of Josephson junctions in a granular superconductor.

3:This research is partly supported by a Cottrell Science Award from Research Corporation.

1:51PM V30.00014 A quadruply twinned core for the growth of nanotetrapods and related structures, S.K. HARK, Z. LIU, The Chinese University of Hong Kong, HARK TEAM — Nanotetrapods and related complex nanoarchitectures, such as multi-armed and tricrystal structures, are key functional elements and interconnections in future “bottom-up” approach to nanotechnology. The growth of these special nanostructures is believed to proceed from a core, several models of have been suggested. However, the occurrence of some tetrapod related nanostuctures, observed by us and also reported by others, can not all be explained by these models. We have obtained aligned ZnCdSe tetrapod related nanostuctures using metalorganic chemical vapor deposition on GaAs substrates. Based on high resolution transmission electron microscopy and crystallographic analyses, we propose a new quadruply-twinned model for their core, from which nanotetrapods, nanowords and related nanoarchitectures can grow. In this model, the core contains four wurtzite structured heptahedrons connected by six (0-113) twins. Different from the other existing models, no polarity of surface is needed to explain the growth of the branching arms of the nanotetrapods.

1The work described in this paper was partially supported by a grant from the Research Grants Council of the Hong Kong Special Administrative Region, China (Project No. 2150521) and CUHK direct grants (Project codes: 2060305).
Ordered layer of Ti for conventional semiconductor interfaces. Density-functional theory calculations including a Hubbard U (LDA+U) have shown that a charge and orbitally that are being incorporated into oxide heterointerfaces offer more degrees of freedom to compensate the charge imbalance at the interface than is the case. 


When oxides meet face to face”. E. Dagotto, Science, 318, 1076 (2007)

Superconducting transitions are consistent with a superconducting sheet as thin as a few nm.

The field effect allows the normal state and superconducting state properties to be spectacularly tuned. The characteristics of the observed superconducting transitions are consistent with a superconducting sheet as thin as a few nm.

Insulating dielectric perovskite oxides. It will be shown that the ground state of this system is superconducting [3]. The superconducting critical temperature is about 200mK. The field effect allows the normal state and superconducting state properties to be spectacularly tuned. The characteristics of the observed superconducting transitions are consistent with a superconducting sheet as thin as a few nm.

1 “When oxides meet face to face”. E. Dagotto, Science, 318, 1076 (2007)


Heterointerfaces$^1$. R. PENTCHEVA, University of Munich, W. PICKETT, University of California Davis — Multivalent transition metal ions that are being incorporated into oxide heterointerfaces offer more degrees of freedom to compensate the charge imbalance at the interface than is the case for conventional semiconductor interfaces. Density-functional theory calculations including a Hubbard U (LDA+U) have shown that a charge and orbitally ordered layer of Ti$^{3+}$ and Ti$^{4+}$ is formed at the interface (IF) between the Mott and the band insulator LaTiO$_3$ (d$^1$) and SrTiO$_3$ (d$^0$) [Phys. Rev. Lett. 99, 016802 (2007)] as well as between the two band insulators LaAlO$_3$ and SrTiO$_3$ [Phys. Rev. B. 74, 035112 (2006)]. Additional complexity relating to charge state and orbital occupation arises at the LaVO$_3$/SrTiO$_3$ interface between these compounds that are d$^2$ and d$^0$ respectively in the bulk: the electron-doped ...-TiO$_2$-LaO... IF may promote a Ti$^{3+}$ charge state, the hole-doped ...-SrO-V-O$_2$-... IF may encourage a V$^{4+}$ ion, or a metallic IF may result. We will present LDA+U predictions of charge states, orbital and spin order, and conducting behavior at these heterointerfaces, and contrast the results with the d$^1$ – d$^0$ and d$^0$ – d$^0$ interfaces mentioned above.

1Supported by a Bavaria California Technology Center grant.

Charge accumulation in nonpolar perovskite quantum well sandwiched by polar Mott-insulating perovskites, CHENG-CHING WANG, University of Texas at Austin, SAHU BHAGAWAN, SWAN, Microelectronics Research Center, HONGKI MIN, WEI-CHENG LEE, MACDONALD ALLAN, H., University of Texas at Austin, CONDENSED MATTER THEORY GROUP AT UT AUSTIN TEAM — We theoretically examine the possibility of having charge accumulation in the (LaTiO$_3$)$_x$/Ba$_2$VO$_4$/LaTiO$_3$$_{1-x}$ layered oxide quantum well system with polar barrier material and non-polar quantum well material using a LDA+U approach. The charge accumulation we find reflects electronic reconstruction which tends to occur near polar/nonpolar heterojunctions. We find enormous orbital reconstruction and both antiferromagnetic and ferromagnetic local in different planes. Lattice relaxation in the structure was allowed as a partial test of the robustness of LDA+U predictions for the properties of this system.

A First Principle Study of the LaAlO$_3$/SrTiO$_3$ Heterointerface, HANGHUI CHEN, Department of Physics, Yale University, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — In order to understand the origin of the intriguing high mobility quasi two dimensional electron gas formed at the LaAlO$_3$/SrTiO$_3$$(001)$ heterointerface, we carry out first principle calculations on the electronic structures and properties of complementary interface. The intrinsic polar properties are investigated and the average electronic potential increase by each LaAlO$_3$ layer is calculated, which can account for the recent observed experiment fact that the heterointerface is not metallic until the number of LaAlO$_3$ layers reaches a critical value. We also study the effects of different surface terminations of SrTiO$_3$ which surprisingly turn out to influence the electronic structure of the interface and so far have not been focused on in experiments.

Electrostatic doping in oxide heterostructures, JAEKWANG LEE, ALEXANDER A. DEMKOV, Department of Physics, The University of Texas at Austin — Recent experiments on perovskite heterostructures grown by molecular beam epitaxy or pulsed laser deposition suggest the possibility of creating high mobility two dimensional electron gas at the oxide/oxide interface. However, the origin of charge in these insulating materials is still not clear and deemed controversial. We report a first-principles study of SrTiO$_3$/LaAlO$_3$ heterostructures using density functional theory at the LDA+U level. We consider the energetics and electronic structure of the junction, while focusing on the role of electrostatics. Our results suggest that a complex balance of the crystal filed, Jahn-Teller effect, lattice dynamics and internal electric field result in the robust electrostatic doping for carefully chosen thickness of the oxide layer. We explore the possible uses of this effect in other oxide-based heterostructures.

KAROLINA JANICKA, JULIAN VELEV, EVGENY TSYMBAI, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA — We perform first-principles electronic structure calculations to elucidate the electronic and magnetic properties of LaAlO$_3$/SrTiO$_3$ and LaTiO$_3$/SrTiO$_3$ superlattices. We find that TiO$_2$-terminated interfaces are n-type conducting which is consistent with experimental observations. In both heterostructures we find that charge resides in Ti conduction band and is localized within a few nanometers from the interface. This charge distribution is consistent with metal induced gap states in the gap of SrTiO$_3$ produced by the interfacial charge. In order to understand the magnetism of these oxide heterostructures, we performed spin-polarized calculations which reveal that this interface in a (LaAlO$_3$)$_n$/(SrTiO$_3$)$_n$ superlattice is magnetic with magnetic moment on the Ti atom. For thicker SrTiO$_3$ layers the magnetism decreases and eventually disappears because the electronic structure of the SrTiO$_3$ substrate is non-magnetic.

For magnetism. The inclusion of electron correlations via the LDA+U approximation with U=5eV on Ti atoms makes the two-dimensional electron gas more localized and half-metallic and strengthens the interface magnetization.

Supported by NSF-MRSEC.

Fabrication and characterization of complex oxide RENiO$_3$/LaAlO$_3$ superlattices

M. KAREEV, University of Arkansas, Fayetteville, J.W. FREELAND, Advance Photon Source, Argonne National Lab., J. LIU, University of Arkansas, Fayetteville, B. KIRBY, NIST, Center for Neutron Research, B. KEIMER, Max Planck Institute for Solid State Research, J. CHAKHALIAN, University of Arkansas, Fayetteville — Nowadays has been growing interest to synthesis of atomically thin complex oxide superlattices which can result in novel electronic and magnetic properties at the interface. Here we report on digital synthesis of single unit cell nickel based heterostructures of RENiO$_3$/LaAlO$_3$ (RE = La, Nd and Pr) superlattices on SrTiO$_3$ and LaAlO$_3$ by laser MBE. RHEED analysis, grazing angle XRD and AFM imaging have confirmed the high quality and chemical homogeneity of the epitaxially grown superlattices. The magnetic and electronic properties of the superlattices have been elucidated by polarized X-ray spectroscopies, which show a non-trivial evolution of magnetism and charge of the LNO layer with increasing LNO layer thickness. The work has been supported by U.S. DOD-ARO under Contract No. 402-17291.

1:03PM V31.00008 Band gap engineering in digital manganese-titanate superlattices

XIAOFANG ZHAI, CHANDRA MOHAPATRA, Department of Physics, University of Illinois at Urbana-Champaign, AMISH SHAH, JIANG-MIN ZHUO, Department of Materials Science Engineering, University of Illinois at Urbana-Champaign, ZORAN POPOVIC, SASHI SATPATHY, Department of Physics, University of Missouri, Columbia, ANAND BHATTACHARYA, Argonne National Lab, JAMES ECKSTEIN, Department of Physics, University of Illinois at Urbana-Champaign — The electronic structure of short period digital superlattices of two different phases depends strongly on the superlattice architecture. We have fabricated digital superlattices of super cells consisting of N layers of LaMnO$_3$ and N layers of SrTiO$_3$, N=1, 2, 3, 8, and measured their optical conductivities to probe the way in which the electronic structure depends on N. We found the valence band structure systematically changes, as N decreases, from bulk like band gaps to modified band gaps. The temperature dependence of the derived Mn Jahn-Teller/Mott gap in large period superlattices is completely different from the small period, suggesting different spin ordering states reside in them. The electronic structure of two parent materials are coherently blended at the interface, and the spin ordering is strongly modified. This method of producing meta materials is a promising new way of material engineering.

1:15PM V31.00009 Charge leakage and effective doping of atomically flat (LaMnO$_3$)$_{2n}$/ (SrMnO$_3$)$_{2n}$ superlattice interfaces

J.J. KAVICH, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, A. BHATTACHARYA, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, M.P. WARUSAWITHANA, Department of Materials Science and Engineering, Penn State University, J.N. ECKSTEIN, Department of Physics, University of Illinois at Urbana-Champaign, Urbana IL 61801 — Atomically flat molecular beam epitaxy (MBE) grown interfaces in high quality digital superlattices provide a unique investigation of the role of substitutional disorder in complex oxide systems. Circularly polarized x-rays are used to measure the electronic and magnetic properties of the random alloy La$_2$/3Sr$_{1}$/3MnO$_3$ as it is digitally ordered into discrete layers of insulating A-type antiferromagnetic LaMnO$_3$ (LMO) and G-type antiferromagnetic SrMnO$_3$ (SMO) with superlattice configurations of (LMO)$_{2n}$/ (SMO)$_{2n}$. The diffusion of carriers across the interface effectively dopes the interface region. The electronic and magnetic structure of the n=1 digital structure is nearly identical to the solid solution of the same doping that shows that, on average, the charge distributes uniformly over the entire sample. The ferromagnetic insulating nature of the n = 5 superlattice suggests a finite lengthscale of the diffusion of carriers at the interface. Work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

1:27PM V31.00010 Structural Basis of Conduction at LaAlO$_3$-SrTiO$_3$ Interfaces

ROY CLARKE, D. KUMAH, C. CIONCA, University of Michigan, P.R. WILLMOTT, Paul Scherrer Institut, Swiss Light Source, S. A. HERGÉR, C.M. SCHLEPUETZ, S.A. PAULI, D. MARTOCCIA, B.D. PATTERSON, B. DELLEY, Paul Scherrer Institut, Y. YACOBY, Hebrew University, Jerusalem — We present new results on the application of the x-ray phase retrieval method, Coherent Bragg Rod Analysis (COBRA), to heterointerfaces in LaAlO$_3$ thin films grown on SrTiO$_3$ substrates, a system known to form an interfacial quasi-2D electronic gas. We observe a doped, mixed-valence interface which modifies the electronic band structure, lowering the minimum of the conduction band below the Fermi level and thereby rendering the doped interface conducting. In particular the COBRA measurements reveal the formation of an interfacial La,SrTiO$_3$ layer with an accumulation of trivalent Ti at the interface which is responsible for the lattice dilatation and minimizes the electrostatic energy at the TiO$_2$-terminated SrTiO$_3$ substrate surface. The work presented here establishes a structural basis for the formation of the conducting interface.

1Supported by Department of Energy, Basic Energy Sciences.

1:39PM V31.00011 Signatures of Enhanced Ordering Temperatures in Digital Superlattices of (LaMnO$_3$)$_m$/(SrMnO$_3$)$_2m$

A. BHATTACHARYA, CNM & MSM, Argonne National Laboratory, S. J. MAY, MSD, Argonne National Laboratory, L. ROBERTSON, HFIR, Oak Ridge National Laboratory, P. RYAN, APS, Argonne National Laboratory, X. ZHAI, J. N. ECKSTEIN, Department of Physics, UIUC, S. D. BADER, CNM & MSM, Argonne National Laboratory — Digital superlattices of (LaMnO$_3$)$_m$/(SrMnO$_3$)$_2m$ for integers m = 1 - 4 have been synthesized with oxygen assisted oxide MBE. These superlattices are ordered analogues of La$_1$/3Sr$_2$/3MnO$_3$, an antiferromagnetic insulator. Signatures of enhanced ordering temperatures have been observed in transport and magnetic measurements. We interpret this in terms of the effects of enhanced A-site order on d$_{x^2-y^2}$ orbital occupancy. We shall also present evidence in support of our findings with x-ray and neutron scattering.

1Supported: DOE-BES Contract # DE-AC02-06CH11357.
1:51PM V31.00012 Nanoscale Control of an Interfacial Metal-Insulator Transition at Room Temperature
   CHENG CEN, JEREMY LEVY, STEFAN THIEL, GERMAN HAMMERL, CHRISTOF W. SCHNEIDER, JOCHEN MANNHART, KRISTOPHER E. ANDERSON, C. STEPHEN HELLBERG — We report the creation and erasure of nanoscale conducting regions at the interface between two insulating oxides, LaAlO$_3$ and SrTiO$_3$. Using voltages applied by an atomic force microscope (AFM) probe, the buried LaAlO$_3$/SrTiO$_3$ interface is locally and reversibly switched between insulating and conducting states. Persistent field effects are observed using the AFM probe as a gate. Patterning of conducting lines with widths $\sim$3 nm, as well as arrays of conducting islands with densities $>10^{14}$/in$^2$, are demonstrated. The patterned structures are stable for $>24$ hours at room temperature.

   C. STEPHEN HELLBERG, Naval Research Lab, KRISTOPHER ANDERSEN, Northern Arizona University, CHENG CEN, JEREMY LEVY, University of Pittsburgh, STEFAN THIEL, GERMAN HAMMERL, CHRISTOF SCHNEIDER, JOCHEN MANNHART, Augsburg University — Although bulk LaAlO$_3$ and SrTiO$_3$ are both insulating, an electron gas can form at the interface between these compounds. For up to 2 unit cells (uc) of LaAlO$_3$, the interface remains insulating, while for 4 uc and beyond, it is metallic. For 3 uc films, the interface can be reversibly switched from metallic to insulating using voltages applied by an atomic force microscope (AFM). We present first-principles density functional calculations of LaAlO$_3$ films on SrTiO$_3$. We show the AFM induced interfacial metal- insulator transition can be explained by the formation and annihilation of oxygen vacancies on the LaAlO$_3$ surface.


11:15AM V32.00001 Structural and chemical ordering and spin polarization in epitaxial films of Co$_x$Mn$_{1-x}$Ge$_1$ and Co$_x$Mn$_{1-x}$Si$_1$-
   1 B.A. COLLINS, L. HE, F. TSUI. University of North Carolina at Chapel Hill, Y.S. CHU, Y. ZHONG, Argonne National Laboratory — The Heusler alloys of Co$_2$MnGe and Co$_2$MnSi have been predicted to be half-metallic. However, half-metallicity has not been realized owing to its sensitivity to disorders associated with off-stoichiometry and to epitaxial constraints. Combinatorial epitaxial films of Co$_x$Mn$_{1-x}$Ge$_1$ and Co$_x$Mn$_{1-x}$Si$_1$ have been grown on Ge (111) substrates in and around the Heusler stoichiometry using molecular beam epitaxy techniques. The structural and chemical ordering of the films has been examined using x-ray microbeam techniques, including energy dependent anomalous diffraction and diffraction anomalous fine structure. These experiments are shown to be sensitive to various disorders, including stacking faults, and chemical dependent vacancies and site swapping. They reveal that the ordering is very sensitive to the atomic ratio between Co and Mn. Magnetic and spin dependent properties have been examined by magneto-optic effects and in-situ point contact Andreev reflection spectroscopy, and they exhibit strong correlation with the structural and chemical ordering.

11:27AM V32.00002 Control of selforganized magnetic nanocrystals aggregation in (Ga,Fe)N by co-doping with shallow donors and acceptors, A. BONANNI, A. NAVARRO-QUEZADA, T. LI. Johannes Kepler University, Linz - Austria, M. KIECANA, M. SAWICKI, T. DIETL, Institute of Physics, PAS - Warsaw — A number of possible room temperature functionalities has recently been proposed for magnetically doped semiconductors, in which spinodal decomposition leads to the self-organized formation of coherent ferromagnetic nanodots or nanocolumns. It has also been suggested that the decomposition can be controlled in a wide range by growth conditions and co-doping. We have extended our previous structural and magnetic studies of (Ga,Fe)N by examining the effects of Si and Mg co-doping. As before, we have found the magnetic response to consist of a paramagnetic signal from substitutional Fe and of a ferromagnetic component due to Fe$_{1-x}$N nanocrystals. Our results demonstrate that the co-doping reduces the fractional concentration of Fe contributing to the nanocrystals. This shows that tuning of the Fermi energy by co-doping with shallow donors and acceptors

11:39AM V32.00003 Giant anisotropic magnetoresistance in ultra thin (Ga,Mn)As, RASHID RASHEED, MARKUS SCHLAPPS, Institute of Experimental and Applied Physics, University of Regensburg, Universitaetsstrasse 31, 93040 Regensburg, Germany, JANUSZ SADOWSKI, MAX-Lab, Lund University, 22100 Lund, Sweden, WERNER WEGSCHEIDER, DIETER WEISS, Institute of Experimental and Applied Physics, University of Regensburg, Universitaetsstrasse 31, 93040 Regensburg, Germany — We describe the effect of giant anisotropic magnetoresistance (GAMR) for epitaxial ultra thin (Ga,Mn)As as below the metal-insulator transition (MIT). The GAMR is observed for 5 nm-thick Ga$_{0.95}$Mn$_{0.05}$As films after annealing in optimized conditions in planar geometry for patterned Hall bars at T<10K, where longitudinal resistance $R_o$~$\eta$ per/2. The GAMR manifests itself in magnetization-dependent high-resistance (HR) and low-resistance (LR) states along different crystallographic directions. We demonstrate that holes are strongly localized in HR states and localization depends on orientation of magnetization, amplitude of current and magnetic field. The decrease of current amplitude is accompanied by an enhancement of the GAMR for both in-plane and orthogonal-to-plane orientations of magnetic field. Changes of $R_o$ between HR and LR states reach~100% at T=1K. In the Hall geometry the changes of transverse component $R_{xy}$ in magnetic field exceed 1000%. The behaviour of GAMR we ascribe to anisotropic spin-orbit scattering, strong localization below MIT and localization-delocalization effects in magnetic and electric fields.

11:51AM V32.00004 Atom-byatom substitution of Mn in GaAs and visualization of their hole-mediated interactions, DALE KITCHEN, Princeton University — No abstract available.
12:27PM V32.00005 Ferromagnetism in CuO-ZnO multilayers. SUKARAN CHANDRAN. Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, B.J. KIRBY. NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, K. PADMANABHAN, G. LAWES, R. NAISK. Department of Physics and Astronomy, Wayne State University, MI 48201, SANJIV KUMAR, NCCCM, Bhaga Atomic Research Centre, ECIL Post, Hyderabad 500062, India, V.M. NAISK. Department of National Sciences, University of Michigan-Dearborn, Dearborn, MI 48128 — The magnetic properties of CuO-ZnO heterostructures are examined to elucidate the origin of the ferromagnetic signature in Cu doped ZnO. The CuO and ZnO layer thickness varied from 15 nm to 350 nm, and we observed no significant diffusion of either Cu$^{2+}$ in the ZnO layers or of Zn$^{2+}$ in the CuO layers using Rutherford backscattering spectrometry. Bulk magnetization measurements established that the multilayers exhibit a ferromagnetic moment at room temperature, with a saturation magnetization (∼2.5 emu/cc of CuO) that depends on the CuO size, but not the CuO-ZnO interfacial area. Polarized neutron reflection studies suggest that the ferromagnetism arises from the CuO layers, and not from the interdiffusion of CuO and ZnO. These results indicate that the ferromagnetism in these multicomponent structures arises from the uncompensated surface spins of CuO nanoparticles in the layer rather than from regions of interdiffusing ZnO and CuO.

12:39PM V32.00006 Role of Donor defects in stabilizing room temperature ferromagnetism in Co doped ZnO. LUBNA SHAH, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, YUAN-QIANG SONG, University of Electronic Science and Technology of China, Chengdu, People’s Republic of China, HUI-LU ZHANG, University of Electronic Science and Technology of China, Chengdu, People’s Republic of China, WEIWANG WANG, ZHU HAO, JOHN XIAO, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716 — Extensive experimental and theoretical work has been done on transition metal doped ZnO diluted magnetic semiconductor, in which defects play a vital role in promoting carrier-mediated ferromagnetism. We explored the influence of interstitial Zinc on physical properties of Co doped ZnO by exposing CuO.5ZnO.5ZO in a Zn vapor. Both X-ray diffraction and X-ray photoelectron spectroscopy indicate the substitution of Co$^{2+}$ in the ZnO lattice. Observed room temperature ferromagnetism in bulk samples shows a decreasing trend with decreasing temperature. This can be explained by taking into the reduction of the carrier density, induced by the interstitial Zinc ions, at low temperature. Carrier density at room temperature is about 8.5 x 10$^{19}$/cm$^3$, which is consistent with predicted value for polaron percolation threshold to induce long range ferromagnetism. The carrier density fell below this threshold at low temperature, results in the disappearance of the ferromagnetism.

12:51PM V32.00007 Ferromagnetism in Rutile Structure Cr doped VO$_2$ Thin Films prepared by Reactive Bias Target Ion Beam Deposition. KEVIN G. WEST, JIWEI LU, LI HE, DAVID M. KIRKWOOD, WEI CHEN, University of Virginia, T. PAUL ADL, Micron Technology, MICHAEL S. OSOFSKY, SYED B. QADRI, US. Naval Research Labs, ROBERT HULL, THOMAS PROFFEN, Manuel WOLF, University of Virginia — First generation spintronics has entered the mainstream of information technology through its utilization of the Magnetic Tunnel Junction (MTJ) in applicable devices such as read head sensors for hard disk drives and Magnetic Random Access Memory (MRAM). The future of spintronics devices requires next generation spintronic materials. Here we report on the novel structural, transport, and magnetic characteristics of V$_1-x$Cr$_x$O$_2$ (0.1 ≤ x ≤ 0.2) thin films deposited on (001) Al$_2$O$_3$ substrates. We show that the metal-insulator transition (MIT) of VO$_2$ is suppressed and the rutile structure is stable down to 100 K. The films are remarkably smooth having a root-mean squared (RMS) surface roughness of 0.3 nm. Films are conductive at room temperature which is consistent with predicted value for polaron percolation threshold to induce long range ferromagnetism. The carrier density fell below this threshold at low temperature, results in the disappearance of the ferromagnetism.

1:03PM V32.00008 Phase transition temperatures and magnetic entropy change in Ni-Mn-In-B based Heusler alloys. ARJUN PATHAK, BHOG AUTAM, IGOR DUBENKO, NAUSHAD ALI, Department of Physics, Southern Illinois University, Carbondale, IL, 62901, MAGNETIC MATERIALS RESEARCH LAB TEAM — One of the aspects of great attention of Heusler alloys is the large value of magnetic entropy change (Δ$S_M$) and their possible application as a working material in magnetocaloric effect based magnetic refrigerators. It was reported earlier that Ni$_{50}$Mn$_{30}$In$_{10}$ has first order martensitic transition temperature $T_M$ ≈ 212K, Curie temperature of austenitic phase $T_C$ ≈ 328K and Δ$S_M$ value associated with $T_M$ and $T_C$ are respectively 15 × 10$^{-3}$ J/kg K$^2$. In the present study, we are reporting the effect of partial substitution of In by B in Ni$_{50}$Mn$_{30}$In$_{10}$ by AC susceptibility, thermal expansion, and magnetization measurements. We observed that substitution of boron sharply increase $T_M$ and significantly enhance the $\Delta S_M$ peak value higher than 30 J/kg K at $T_M$ ≈ 296K; however the $\Delta S_M$ value remains almost same at $T_C$. Therefore, the Ni-Mn-In-B based Heusler alloys will be potential material for room temperature magnetic refrigeration materials. Reference: [1] A. K. Pathak, M. Khan, I. Dubenko, S. Stadler, and N. Ali, Appl. Phys. Lett. 90, 262504 (2007).

1:15PM V32.00009 Magnetic excitations in a quantum spin dimer system Ba$_2$Cr$_2$O$_8$. MAIKO KOFUJ, JUNG-HWA KIM, SEUNG-HUN LEE, Univ. of Virginia, BELLA LAKE, Hahn-Meitner Institute, YIMING QIU, National Institute of Standards and Technology, HIROKI UEDA, YUTAKA UEDA, JISSP, Univ. of Tokyo — We report our neutron scattering measurements on a powder sample of a new quantum spin system Ba$_2$Cr$_2$O$_8$. Spin-lattice coupling and exchange interactions are probed using inelastic neutron scattering measurements probing energy transfers to 50 mK. Instead, bulk susceptibility data exhibit a broad peak around 16K. Our inelastic neutron scattering data at temperatures lower than 30 K show a prominent excitation at hw = 2.2 meV. Q- and temperature dependences of the integrated intensity of the excitation can be well accounted for by a model of weakly coupled quantum dimers. When an external magnetic field is applied, the excitation splits into three energies, which confirms the dimer model. We have investigated how the singlet-to-triplet excitations evolve with increasing the magnetic field up to 14.5 Tesla.

1:27PM V32.00010 Understanding Magnetic Frustration on the Diamond Lattice of Transition Metal Oxide Spinel. BRENT MELOT, KATHARINE PAGE, RAM SESHADRI, Materials Department, University of California, Santa Barbara, CA, 93106–5050 USA, DORON BERGMAN, Physics Department, University of California, Santa Barbara, CA, 93106–9530 USA, THOMAS PROFFEN, Manuel Lujan, Jr. Neutron Scattering Center, Los Alamos National Laboratory, LANSE-12, MS H805, Los Alamos, New Mexico 87545, USA — We present structural and magnetic measurements on the cubic spinel perovskite CuO$_2$Rh$_2$O$_6$(Al$_{1-x}$Ga$_x$O$_{2-x}$) and demonstrate how frustration on the diamond sublattice can be modified through chemical substitution. The effect of substitution is two-fold. Increasing values of $x$ are accompanied by an increase in the lattice parameter resulting in an elongated and consequentially weakened exchange pathway. Our data indicates that the amount of site mixing also increases across the substitution series weakening the A-O-B-O-A superexchange pathway. Monte Carlo simulations were used to compute the exchange coupling constants between nearest and next-nearest neighbor Co atoms. Density functional calculations were also performed to approximate the nearest neighbor coupling constant. For most values of $x$, we find that the frustration parameter, $\Theta_{CW}/T_N$, decreases which we attribute to the weakening competition between nearest and next-nearest-neighbor Co exchange interactions.

1:39PM V32.00011 Half-metallic Silicon Nanowires. EGIN DURGUN, DENIZ CAKIR, NURTEN AKMAN, SALIM CIRACI — This study investigates the atomic structure, mechanical, electronic and magnetic properties of silicon nanowires using first-principles plane wave calculations within density functional theory. We considered bare, hydrogen terminated and transition-metal adsorbed silicon nanowires oriented along [001] direction. Nanowires of different sizes are initially cut from the bulk Si crystal in rod-like forms and subsequently their atomic structures are relaxed. We first present an extensive analysis of the atomic structure, stability, elastic and electronic properties of bare silicon nanowires. The energetics of adsorption and resulting electronic and magnetic properties are examined for different levels of transition metal atom coverage. Adsorption of transition metal atoms resulted in magnetic ground state. The net magnetic moment increases with increasing coverage. While specific Si nanowires acquire half-metallic behavior at low coverage, at high coverage ferromagnetic nanowires become metallic for both spin-direction and some of them have very high spin polarization at the Fermi level. Present results are not only of scientific interest, but can also initiate new research on spintronic applications of silicon nanowires. [1] E.Durgun, D. Cakir, N. Akman and S. Ciraci, Phys. Rev. Lett (2007) (in press).
waves and high frequency electron paramagnetic resonance, STEPHEN HILL, JONATHAN LAWRENCE, Department of Physics, University of Florida, FERRAN MACIA, JOAN MANEL HERNANDEZ, JAVIER TEJADA, Departament de Fisica Fonamental, University of Barcelona, PAULO SANTOS, Paul-Drude-Institut, Berlin, CHRISTOS LAMPROPOULOS, GEORGE CHRISTOU, Department of Chemistry, University of Florida — We report a new experimental technique that integrates high frequency surface acoustic waves (SAWs) with high frequency electron paramagnetic resonance (HFEP) spectroscopy in order to measure spin dynamics on fast time scales in single-molecule magnets. After driving the system out of equilibrium by triggering magnetic avalanches, or simply by heating with short SAW pulses, the evolution of the spin populations within fixed energy levels is measured using HFEP spectroscopy.

Thursday, March 13, 2008 11:15AM - 2:15PM –
Session V33 GMAG FIAP DMP: Focus Session: Theory of Spin Phenomena in Semiconductors
Morial Convention Center 224

11:15AM V33.00001 Design of dilute magnetic semiconductors with room temperature ferromagnetism by controlling spinodal decomposition1. KAZUNORI SATO, ISIR, Osaka University — Owing to the recent development of the first-principles method for calculating magnetic properties of dilute magnetic semiconductors (DMS), it has been recognized that the magnetic percolation effect is disastrous to the high temperature ferromagnetism in DMS in particular for low concentrations [1]. The exchange interactions calculated from first-principles are strong for nearest neighbors, but those interactions are short ranged and can not play an important role for realizing high-\(T_C\) because the solubility of magnetic impurities into DMS is too low to achieve magnetic percolation. To overcome this difficulty and realize room temperature ferromagnetism, we focus on the spinodal decomposition in DMS, and suggest that by controlling the spinodal decomposition high blocking temperature can be realized leading to ferromagnetic behaviour at high temperature [2]. We calculate electronic structure of DMS from first-principles by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. Then, chemical pair interactions and magnetic exchange interactions between magnetic are calculated. We use the Monte Carlo techniques to simulate spinodal decomposition of DMS and to estimate the magnetic properties of them [3]. The computer simulations for the magnetization process of the decomposition phases indicate that we can control super-paramagnetic blocking temperature by optimizing the size of the clusters by changing the crystal growth condition. This simulation suggests the material design of high blocking temperature DMS by controlling the spinodal decomposition [2]. As another approach for realizing high-\(T_C\) DMS we propose co-doping method to increase solubility limit of transition metal impurities in DMS [4]. This work is based on the collaboration with H. Katayama-Yoshida and T. Fukushima.

1 This work was partially supported by a Grant-in-Aid for Scientific Research in Priority Areas “Quantum Simulators and Quantum Design” (No. 17064014) and a Grand-in-Aid for Scientific Research for young researchers and the Kansai Research Foundation.

11:51AM V33.00002 Defect-induced intrinsic magnetism in wide-gap III-nitrides1. PEIHONG ZHANG, PRATIBHA DEV, YU XUE, University at Buffalo, SUNY — Cation vacancy induced Intrinsic magnetism in GaN and BN is investigated by employing density functional theory based electronic structure methods. The strong localization of defect states favors spontaneous spin polarization and local moment formation. A neutral cation vacancy in Ga\(_2\)N or BN leads to the formation of a net moment of 3\(\mu_B\) with a spin-polarization energy of about 0.5 eV at the low density limit. The extended tails of defect wavefunctions, on the other hand, mediate surprisingly long-range magnetic interactions between the defect-induced moments. This duality of defect states suggests the existence of defect induced or mediated collective magnetism in these otherwise nonmagnetic sp systems.

1 We acknowledge the computational support provided by the Center for Computational.

12:03PM V33.00003 Design of Colossal Solubility of Magnetic Impurities for Semiconductor Spintronics by the Co-doping Method1. TETSUYA FUKUSHIMA, ISIR, Osaka University, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA — Based on first-principles calculations, we propose co-doping method for increasing solubility of magnetic impurities in dilute magnetic semiconductors (DMSs). The concentration dependences of the mixing energy of DMS, such as (Ga,Mn)N, (Ga,Cr)N, (Ga,Mn)As, and (Zn,Cr)Te, show large convexity and these systems have a tendency toward spinodal decomposition. By introducing compensating impurities into these DMS, the mixing energy shows gradual transition from convex to concave concentration dependence resulting in negative mixing energy of magnetic impurities. This observation suggests that the co-doping method dramatically increases the solubility of magnetic impurities in DMS, thus high concentration doping of magnetic impurities into DMS becomes possible.

1 a Grant-in-Aid for Scientific Research on Priority Areas and a Grant-in-Aid for Specially Promoted Research.
12:15PM V33.00004 Suppression of ferromagnetism in Zn$_x$Cr$_{1-x}$Te: A DFT study , JUAREZ L.F. DA SILVA, National Renewable Energy Lab, 1617 Cole Blvd., Golden, CO 80401, USA; GUSTAVO M. DALPIAN, Centro de Ciencias Naturales e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil; SU-HUI WANG, National Renewable Energy Lab, 1617 Cole Blvd., Golden, CO 80401, USA — The possibility to control the charge and spin degrees of freedom independently in diluted magnetic semiconductors (DMS) provides an opportunity in the realization of spintronic devices. Therefore, there is a great desire to understand the physical parameters that control $T_C$ in DMS. In this talk, we will report a density functional theory study of Zn$_x$Cr$_{1-x}$Te and Ga$_x$Cr$_{1-x}$As, which show interesting carrier dependence of the $T_C$. We found that the stability of ferromagnetism (FM), which is calculated with respect the anti-ferromagnetic (AFM) phase, can be controlled by $n$- and $p$-type co-doping. For randomly distributed Cr, the maximum FM stability is found to be at $\approx 1.25$ holes per magnetic ion. Furthermore, we studied the formation of magnetic Cr precipitates by analysing the binding energy of two Cr atoms in the host semiconductors. Our results indicate that a simple Coulomb binding picture cannot provide a consistent explanation for the formation of Cr-rich aggregates. Instead, we show the variation of Cr-Cr binding energy can be described quite well using the band coupling model [G. M. Dalpian, S.-H. Wei, A. J. R. da Silva, and A. Fazzio, Solid State Commun. 138, 353 (2006)].

12:27PM V33.00005 Eight-band model of the dilute magnetic semiconductor GaMnAs, A. NILI, University of Cincinnati, M. A. MAJIDI, J. MORENO, University of North Dakota, P. KENT, Oak Ridge National Laboratory, M. JARRELL, University of Cincinnati — The ordered state of GaAs doped with Mn is studied using a self-consistent Dynamical Mean Field treatment parameterized with the LDA band structure of the parent material. The resulting model is an eight-band $k$-$p$ model including the heavy and light valence bands, the split-off valence band and the conduction band. The interaction between randomly distributed magnetic ions and itinerant charge carriers is modeled with a modified double-exchange coupling, which includes the attractive potential between holes and charged magnetic ions. Since our method is not perturbative we can treat both strong and weak coupling regimes. We calculate the transition temperature, the temperature dependence of the local magnetization, the density of states and the spin polarization of the holes. We compare our results with more simplified models.

12:39PM V33.00006 Spin relaxation of two-dimensional excitons in a strong magnetic field, O. OLENDLSKI, T. V. SHAHBAZIAN, Jackson State University — We study spin relaxation of quantum well excitons in a perpendicular magnetic field. We show that in a strong field, the dominant relaxation mechanism for an optically-excited magnetoexciton is phonon-assisted spin-orbit transition of the constituent electron or hole. We calculate relaxation rates for excitons in GaAs quantum wells excited by both left and right-polarized light and find that they are much slower than those in quantum dots due to the dominant contribution of exciton kinetic energy in the final state. We also find that the relaxation rate is very sensitive to the applied in-plane electric field that causes exciton drift in the ground state.

1Supported by NSF

12:51PM V33.00007 Theory of exchange splittings of bands in diluted magnetic semiconductors, TOMASZ DIETL, CEZARY SLIW, Institute of Physics, PAS, Warsaw — A series of recent photoemission and magnetooptical experiments, particularly on magnetically doped nitrides and oxides, but also on (Ga,Mn)As, points to the limiting understanding of the physics governing the sp-d exchange interaction in these systems. We have developed theory of band splittings in diluted magnetic semiconductors taking into consideration a possibility that the magnetic ion can trap a hole. We have found that the exchange coupling between the bound and delocalized carriers has actually a similar magnitude to that characterizing the sp-d exchange. Furthermore, our results demonstrate that the presence of the conduction band state itself renormalizes extended states in a spin-dependent fashion. We show that these two effects can explain the unexpected sign and magnitude of the apparent s- d and p-d exchange integrals determined by magneto optical studies carried out for (Ga,Mn)As [3] as well as for (Zn,Co)O, (Ga,Mn)N, and (Ga,Fe)N [4].


1supported partly by JST ERATO project and EC NANOSPIN project

1:03PM V33.00008 Computational materials Design for Spin-Currents Control in Semiconductor Nano-spintronics, HIROSHI KATAYAMA-YOSHIDA, TETSUYA FUKUSHIMA, VAN AN DIENG, KAZUNORI SATO, ISIR, Osaka University — We design the different exchange mechanism like Zener’s double exchange, Zener’s p-d exchange and super-exchange in dilute magnetic semiconductors (DMS) by ab initio calculations. We obtain a universal trend for the exchange interactions [1]. We show that self-organized spinodal nano-decomposition (Dainiaki-Phase) offers the functionality to have high Curie temperatures [2]. We show that spinodal nano-decomposition under layer-by-layer crystal growth condition (2D) leads to quasi-one dimensional nano-structures (Konbu-Phase) with highly anisotropic shape and high $T_C$ [2]. We design a spin-currents-controlled 100 Tera bits/inch$^2$, Tera Hz switching, and non-volatile MRAM based on Konbu-Phase [2]. In addition to the conventional Peltier effect, we propose a colossal thermoelectric cooling power based on the adiabatic spin-entropy expansion in a Konbu-Phase [3]. [1] B. Belhadj et al., J. Phys.-Condens. Matter, 19 (2007) 436227. [2] H. Katayama-Yoshida et al., Phys. stat. sol. (a) 204 (2007) 15. [3] H. Katayama-Yoshida et al., Jpn. J. Appl. Phys. 46 (2007) L777.

1This work was partially supported by Grant-in-Aid for Scientific Research in Priority Areas and for Specially Promoted Research.

1:15PM V33.00009 Effect of Fermi level on Microstructure and Magnetism in (Ga,Mn)N Alloys, JENNIFER CHAN, ZHELIU, STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — GaN doped with Mn has been shown experimentally to exhibit either ferro- or antiferro- magnetic behavior, the results varying considerably depending on the microstructure of the sample. Indeed, the electronic structure and magnetic properties appear to be heavily dependent upon growth conditions and ordering of the material. We used ab-initio calculations to investigate the magnetism of various ordered structures of (Ga,Mn)N with respect to Mn composition. The results show that high-spin states with the spins on the Mn aligned in parallel (HS-FM) are stable at low Mn composition ($< 0.5\%$) but not at high Mn composition ($> 5\%$). Instead, for high Mn composition, low-spin states (LS-FM) or states where the spins on the Mn are anti-parallel (FI) are found. Interestingly, upon raising the Fermi level, the HS-FM states are stable for all Mn compositions and their formation enthalpies lower with respect to the neutral Fermi level case indicating that electron doping leads to enhanced Mn solubility and hence charged microstructure. The short and long range ordering, tendency for clustering and magnetic properties will be investigated.

1Funded by DARPA under NREL contract No. DE-AC36-99GO10337
1:27PM V33.00010 First-Principles Study on Electronic Structure of TiO$_2$-Based Dilute Magnetic Semiconductors$^1$, HIDETOSHI KIZAKI, MASAYUKI TOYODA, AZUMUNI SATO, HIROSHI KATAYAMA-YOSHIDA — We investigate the electronic structure in rutile-TiO$_2$-based dilute magnetic semiconductors (DMS) within self-interaction-corrected local density approximation (SIC-LDA). These results are compared with those calculated within standard LDA. Although the calculated band-gap energy and energetic position of Ti 3$d$ bands are different in the LDA and the SIC-LDA, half-metallic density of states is predicted in transition-metal-doped TiO$_2$ for both methods. While the LDA calculations predict high-spin state only for Fe-doped one, in the SIC-LDA calculations high-spin state is realized in V-, Cr- and Mn-doped one and low-spin state is realized in Fe- and Co-doped one. However, the absorption and soft x-ray magnetic circular dichroism measurements in (Ti$_{100-x}$Co$_x$)$_2$O$_2$ indicate the Co$^{2+}$ high-spin state in the $D_{2d}$-symmetry crystal field at the Ti site. These experimental results do not agree with our calculated results. We will discuss the origin of the discrepancy between the theoretical predictions and the experimental observations. In addition, we will discuss the ferromagnetism in TiO$_2$-based DMS.

$^1$This work was partially supported by a Grant-in-Aid for Scientific Research in Priority Areas and for specially promoted research

1:39PM V33.00011 Ferromagnetism in GaN:Gd: A density functional theory study$^1$, LEI LIU, LBNL, UCB, PETER YU, UCB, LBNL, Z.X. MA, LBNL, SAM MAO, LBNL, UCB — First principle calculations of the electronic structure and magnetic interaction of GaN:Gd have been performed within the Generalized Gradient Approximation (GGA) of the density functional theory (DFT) with the on-site Coulomb energy $U$ taken into account (also referred to as GGA+$U$). The magnetic $p-d$ coupling is found to be over two orders of magnitude larger than the $d-d$ exchange coupling. The experimental collosal magnetic moments and room temperature ferromagnetism in GaN:Gd reported recently are explained by the interaction of Gd 4$f$ spins via $p-d$ coupling involving holes introduced by intrinsic defects such as Ga vacancies.

$^1$Supported by the U.S. Department of Energy. NNSA/NA-22, under Contract No. DE-AC02-06CH11231.

1:51PM V33.00012 Thermodynamics of carrier-mediated magnetism in semiconductors$^1$, A.G. PETUKHOV, South Florida School of Mines and Technology, Rapid City, L. MAKINISTIAN, South Dakota School of Mines and Technology (on leave from CONICET, FI-UNER, Argentina), S.C. ERWIN, Naval Research Laboratory, R. ABOLFATH, University of Texas Southwestern, I. ZUTIC, SUNY Buffalo — We propose a model of carrier-mediated ferromagnetism in semiconductors that accounts for the temperature dependence of the carrier population. The model permits an analysis of the thermodynamic stability of competing magnetic states, opening the door to the construction of magnetic phase diagrams. As an example we analyze the stability of a possible room-temperature ferromagnetic semiconductor, in which temperature leads to an increased carrier density, such that the enhanced exchange coupling between magnetic impurities results in the onset of ferromagnetism as temperature is raised. We apply this approach to studying the thermodynamic fluctuations of magnetization in small systems such as bound magnetic polarons and magnetic nanolands.

$^1$Supported by US ONR, NSF-ECCS and CAREER.


2:03PM V33.00013 Electronic structure and magnetism of Fe$_{1-x}$Mn$_x$N compounds, LI CHEN, Tulane University, TULANE UNIVERSITY TEAM, LINYI NORMAL UNIVERSITY TEAM — The electronic structure and magnetism of Fe$_{1-x}$Mn$_x$N compounds have been studied by a periodic-quantum-mechanical calculation based on density functional theory. The results show that a ferromagnetic ordered phase is stable when Fe is substituted by Mn on cube corner sites, whereas the antiferromagnetic phase is energetically favored when Mn substitutes for Fe on face-centered sites. Mn atom concentration and the substitutional sites have significant influence on the exchange coupling. We predict covalent bonds between face-centered Fe or Mn 3$d$ and N 2$p$ orbitals. In contrast, bonding between the atoms at cube corners and face-centered sites is mainly ionic or metallic.


11:15AM V34.00001 Session Introduction, BEVERLY HARTLLINE, Delaware State University — This abstract not available.

11:25AM V34.00002 The APS 2007 Meeting on Gender Equity in Physics, ARTHUR BIENENSTOCK, Stanford University — This abstract not available.

11:44AM V34.00003 Promoting Positive Images of Women in Physics, BARBARA SANDOW — Why are so few women among the students who study physics? Worldwide statistics show that there have been very few female students in the physics in any country, in the past and in current times. The situation in Germany is outstandingly precarious. The fraction of women to study physics is lower than 15% of all students of the activities in Germany and in other countries. The aims are to bring more girls in to physics, modify the image of scientists and find ways to stop women from dropping out of physics. The experiences and the expectations will be discussed.

12:03PM V34.00004 She’s a Physicist!$^1$, LAURA H. GREENE, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801 USA — Any minority often feels either left out or at the center of attention. The difficulty of blending in creates both challenging obstacles and unique opportunities. Such negative and positive distractions, whether major or minor, can have a profound impact on accomplishing one’s goals. Success requires sustained focus, a constant eye on the “big picture”, and the ever-important sense of humor. In other words, don’t be distracted by the ups and downs, keep your passion focused on the science, and enjoy the ironies. I will discuss some of my personal experiences as a woman and how I have learned to navigate the physics world since before 1970. Through losses and wins, I will share how I have managed to, at least most of the time, keep on keeping on.

$^1$I presently enjoy funding from the U.S. DoE Division of Materials Sciences DE-FG02-07ER46453 through the FSMRL, the NSF DMR 07-06013, and continual support from my sisters and girlfriends
12:22PM V34.00005 Women in Physics in a Rapidly Changing China — LING-AN WU, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China — Despite the upheavals of the 20th century, physics managed to survive quite well in China, where the first woman president of the American Physical Society was born and bred. During the 1950s as a result of policies that emphasized science and engineering, declared equal rights and equal pay for men and women, and assigned jobs to college graduates irrespective of sex, the number of women in physics increased rapidly, many of whom made notable achievements. Since China’s opening up over the last thirty years tremendous changes have taken place, and women now face new opportunities as well as challenges in all aspects of society. Whereas physics used to be regarded as the most elite of the sciences, new fields such as computer science, biotechnology and business are now competing for the best students. Compared with other countries the statistics are not bad; in schools and many physics departments the ratio of women teachers may be 30% or higher, but the numbers drop drastically with rank. Moreover, in some research institutions the ratio of female physicists is actually declining, due to retirement of the older generation and fewer successors. Compulsory retirement for women at an earlier age than for men is also a new factor. Conversely, in recent years the ratio of female graduate students enrolling in physics has increased, even reaching 40% in some universities. However, the reasons for this do not bode well: men are not performing so well as women in entrance exams, while the latter are facing increasing discrimination in employment so they have to seek higher degree qualifications. With the further development of China’s economy there will be abundant demand for qualified personnel including women with a physics background. It is imperative to actively support the upcoming generation of women physicists and not lose them in the leaky pipeline. The Chinese Physical Society has taken certain positive steps, such as the recent establishment of the Xie Xi-De Prize for Women in Physics. However, there is complacency and a general lack of awareness of the special difficulties and discrimination that women in physics face, and this needs to be brought to the attention of all sectors at all levels.

12:41PM V34.00006 Marshak Lectureship Talk: Women in Physics in the Baltic States Region: Problems and Solutions — DALIA SATKOVSKIENE, Vilnius University — In this contribution the gender equality problem in physics will be discussed on the basis of the results obtained implementing the project “Baltic States Network: Women in Sciences and High Technology” (BASNET) initiated by Lithuanian women physicists and financed by European Commission. The main goal of BASNET project was creation of the regional Strategy how to deal with women in sciences problem in the Baltic States. It has some stages and the contribution follows them. The first one was in depth sociological study aiming to find out disincentives and barriers women scientists face in their career and work at science and higher education institutions. Analysis of results revealed wide range of problems concerned with science organization, management and financing common for both counterparts. However it also proved the existence of women discrimination in sciences. As main factors influencing women under-representation in Physics was found: the stereotypes existing in the society where physics is assigned to the masculine area of activity; failings of the science management system, where highest positions are distributed not using the institutionalized objective criteria but by voting, where the correctness of majority solutions is anticipated implicitly. In physics where male scientists are the majority (they also usually compose executive boards, committees etc.) results of such a procedures often are unfavorable for women. The same reasons also influence women “visibility” in physicist’s community and as the consequence possibility to receive needed recourses for their research as well as appropriate presentation of results obtained. The study revealed also the conservatism of scientific community- reluctance to face existing in the scientific society problems and to start solving them. On the basis of the results obtained as well practice of other countries the common strategy of solving women in physics (sciences) in the Baltic States region was formulated. As changing the stereotypes is long lasting process it was decided firstly to concentrate strategy implementation plans on changes in science management policy tackling the problem from the top and allowing receive the most quick results. For this we created the regional Baltic States Network among the corresponding international women working groups, professional organizations (Scientific societies) and corresponding departments of the governmental institutions. BASNET also became a full member of European Platform of Women Scientists (EPWS)-prestige women organization signally influencing the European Community science policy.

1:15PM V34.00007 Panel Discussion —
Thursday, March 13, 2008 11:15 AM - 2:03 PM —
Session V35 DMP FIAP: Focus Session: Thermoelectric Phenomena in Nanostructured Materials Morial Convention Center 227

11:15AM V35.00001 Thermoelectric Properties of Complex Zintl Phases — G. JEFFREY SNYDER, California Institute of Technology — Complex Zintl phases make ideal thermoelectric materials because they can exhibit the necessary “electron-crystal, phonon-glass” properties required for high thermoelectric efficiency. Complex crystal structures can lead to high thermoelectric figure of merit (zT) by having extraordinarily low lattice thermal conductivity. A recent example is the discovery that Yb$_{11}$MnSb$_{11}$, a complex Zintl compound, has twice the zT as the SiGe based material currently in use at NASA. The high temperature (300K - 1300K) electronic properties of Yb$_{11}$MnSb$_{11}$ can be understood using models for heavily doped semiconductors. The free hole concentration, confirmed by Hall effect measurements, is set by the electron counting rules of Zintl and the valence of the transition metal (Mn$^{1+2}$). Substitution of nonmagnetic Zn$^{1+2}$ for the magnetic Mn$^{1+2}$ reduces the spin-disorder scattering and leads to increased zT (10%). The reduction of spin-disorder scattering is consistent with the picture of Yb$_{11}$MnSb$_{11}$ as an underscreened Kondo lattice as derived from low temperature measurements. The hole concentration can be reduced by the substitution of Al$^{1+2}$ for Mn$^{1+2}$, which leads to an increase in the Seebeck coefficient and electrical resistivity consistent with models for degenerate semiconductors. This leads to further improvements (about 25%) in zT and a reduction in the temperature where the zT peaks. The peak in zT is due to the onset of minority carrier conduction and can be correlated with reduction in Seebeck coefficient, increase in electrical conductivity and increase in thermal conductivity due to bipolar thermal conduction.

11:51AM V35.00002 A theoretical study of thermoelectric metamaterial1 — JIANWEI CAI, GERALD MAHAN, Department of Physics, Penn State University — An artificial crystalline material with nanoparticles connected by conducting linkers is proposed for thermoelectric application. Such materials can be synthesized with chemical approaches. The advantage of such materials for thermoelectric application will be discussed. A simple theoretical model for such materials is proposed. Basic theoretical results about the band and properties of the materials based on perturbation theory will be presented.

1Work funded by NSF DMR-0213623 and the Pennsylvania Ben Franklin Technology Development Fund.

12:03PM V35.00003 High Thermoelectric Performance of Nanostructured Bismuth Telluride Bulk Alloys — B. POUDEL, Q. HAO, Y. MA, A. MINNICH, A. MUTO, Y.C. LAN, B. YU, X. YAN, D.Z. WANG, D. VASHAAE, X.Y. CHEN, M.S. DRESSELHAUS, G. CHEN, Z.F. REN, GMZ ENERGY, INC. TEAM, DEPARTMENT OF PHYSICS, BOSTON COLLEGE TEAM, DEPARTMENT OF MECHANICAL ENGINEERING, DEPARTMENT OF PHYSICS, MIT COLLABORATION — Bismuth Telluride and its alloys are best thermoelectric materials for near room temperature applications like refrigeration and waste heat recovery. We have been pursuing an approach of random nanostructures in bulk to improve ZT of these materials. Here we report that ZT values of these random nanostructured materials were improved significantly over the state-of-the-art values. Experimental data coupled with microstructure studies and modeling shows that the ZT improvement mainly comes from a lower thermal conductivity because of the increased phonon scattering by defects and grain boundaries. Significantly improved power generation and cooling data produced from these samples confirmed the high ZT values.

1Supported partly by DOE and NSF.
The Effect of Bi/Sb ratio on Maximum ZT in Nanostructured p-type Bi$_2$Sb$_2$-Te$_3$ Alloys, YI MA, BO YU, BED POUDEL, YUCHENG LAN, JIAN YANG, ZHIFENG REN, Physics Dept., Boston College, QING HAO, GANG CHEN, Department of Mechanical, Massachusetts Institute of Technology — Alloy nanoparticles Bi-Sb$_2$-Te$_3$ (x = 0.2, 0.3, 0.4, 0.5 and 0.6) were synthesized from bismuth, antimony, and tellurium and compacted into nanostructured bulk samples with full density. The thermoelectric properties were measured in the temperature range of 25 to 250°C. We showed that a maximum dimensionless figure-of-merit (ZT) reached 1.27 at about 100°C for Bi$_{0.4}$Sb$_{1.6}$Te$_3$ (x = 0.4), a significant improvement over the state-of-the-art p-type Bi$_2$Te$_3$ alloys. It is demonstrated that the enhanced ZT mainly comes from a reduced thermal conductivity due to the increased phonon scattering due to the nano size of the grains. Also, the ZT peaks shift from low temperature to high temperature with the decreasing of x, which indicates the less Bi content would benefit the potential power generation application while the more Bi content materials could be used as a potential cooling device. This new route of enhancing ZT value can be applied to other materials.

XAS study of Bi$_2$Te$_3$/Sb$_2$Te$_3$ Superlattices and Sb$_{1.5}$Bi$_{0.5}$Te$_3$ Alloy Film, AZZAM MANSOUR, NSWC, Carderock Division, RAY VENKATASUBRAMANIAN, RTI International — Bi$_2$Te$_3$/Sb$_2$Te$_3$ superlattices are being developed for high performance thermoelectric devices. We have used X-ray absorption spectroscopy (XAS) to investigate the local structure of Sb in 20/40 Å and 10/50 Å Bi$_2$Te$_3$/Sb$_2$Te$_3$ superlattices, a Sb$_2$Bi$_2$Te$_6$ alloy film, and a Sb$_2$Te$_3$ reference film. The films were grown on GaAs using a novel low temperature metal-organic chemical vapor deposition method. Initially, we evaluated the local structure parameters of Sb in the superlattices and the alloy relative to those of the reference Sb$_2$Te$_3$ film. Using temperature dependent Sb K-edge XAS measurements, we were able to separate structural disorder from thermal disorder for the Sb-Te pair. The temperature dependence of thermal disorder was analyzed using the Einstein and Debye models for lattice vibrations. A comparison of the results for the superlattices, the alloy and the reference film will be made. The goal is to identify key structural factors that may contribute to the enhanced value of the figure of merit “ZT” and, hence, the improved conversion efficiency for the superlattices relative to the alloys.

Thermoelectric properties of PbTe/PbSe mesomaterials, FENG CHEN, YAOI WANG, YUNI XUE, C. W. CHU, Dept. of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX 77204-5002, JUN ZHANG, JIE FANG, Dept. of Chemistry, State University of New York at Binghamton, Binghamton, NY 13902-6000, CHUNHUI TAN, ZHIFANG LIN, BOB LUL, Aegis Technology, Inc., 3300A Westminster Ave., Santa Ana, CA 92703 — Ball milled PbTe mixed with PbSe nano-wires (PTSW) or with PbSe nano-crystals (PTSC) are sintered under high pressure. Different sintering conditions are tested to preserve the mesostructures. Thermoelectric properties (resistivity, Seebeck coefficient and thermal conductivity) are measured at various temperatures. Pure ball milled PbTe are also sintered and measured for comparison. In this talk, we will present these data and compare with various PbTe data from the literature. Our results show that this mesostructure approach is promising and the sintering condition is the key factor for further improvement.

Transport Properties of Lead Chalcogenide Nanocomposites, GEORGE NOLAS, JOSHUA MARTIN, STEVE STEFANOSKI, Department of Physics, University of South Florida, Tampa, FL, USA, LI WANG, LIDONG CHEN, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China, UNIVERSITY OF SOUTH FLORIDA TEAM, SHANGHAI INSTITUTE OF CERAMICS TEAM — Lead chalcogenide dimensional nanocomposites were prepared by densifying nanocrystals, synthesized in high purity - high product yield employing an alkaline aqueous solution-phase reaction, by Spark Plasma Sintering. Transport properties were evaluated through temperature dependent resistivity, Hall, thermopower, and thermal conductivity measurements. The physical properties of these materials are strongly sensitive to stoichiometry, doping, and porosity. The transport properties of the nanocomposites were compared to that of bulk polycrystalline materials with similar compositions and carrier concentrations. An enhancement of the room temperature thermoelectric properties of up to 30% over that of the bulk was realized.

Nanostructured thermoelectric skutterudite Co$_{1-x}$Ni$_x$Sb$_3$ alloys, QINYU HE, Boston College, South China Normal University, XIAOWEI WANG, JIAN YANG, YUCHENG LAN, XIAO YAN, BO YU, YI MA, BED POUDEL, GIRI JOSHI, DEZHI WANG, ZHIFENG REN, Boston College, QING HAO, GANG CHEN, MIT, BOSTON COLLEGE, REN’S LAB COLLABORATION, MIT COLLABORATION, SOUTH CHINA NORMAL UNIVERSITY COLLABORATION — Nanostructured Ni-doped skutterudites Co$_{1-x}$Ni$_x$Sb$_3$ (with x ranging from 0.01 to 0.09) have been prepared by ball-milling and direct-current induced hot press. It was found that the thermal conductivity was much reduced due to strong electrons-phonons scattering from Ni-doping and grain boundary phonons scattering from nano-structures in the samples. A maximum dimensionless figure-of-merit of 0.71 has been obtained in Co$_{0.91}$Ni$_{0.09}$Sb$_3$ at 525 °C.

Correspondence author

Thermal conductivity reduction by interface roughness in AlN$_x$-GaN$_y$ superlattices, YEE KAN KOH, Univ of Illinois at Urbana-Champaign, YU CAO, Univ of Notre Dame, DAVID CAHILL, Univ of Illinois at Urbana-Champaign, DEBDEEP JENA, Univ of Notre Dame — A reduction of cross-plane thermal conductivity by a factor of two is achieved in AlN$_{12.4}$-GaN$_{25.6}$ superlattices by varying the plasma power during growth. This reduction is attributed to interface roughness, introducing a new parameter to be considered in the design and fabrication of superlattices for thermoelectric applications. Thermal conductivity of AlN$_{12.4}$-GaN$_{25.6}$ superlattices, x ~ 4 nm and 2 < y < 1000 nm, with rough interfaces is then measured by time-domain thermoreflectance. A decreases monotonically as the GaN thickness y decreases, $\Delta = 6.35$ W m$^{-1}$ K$^{-1}$ at y = 2.2 nm. We observe no minimum thermal conductivity as a function of period for these rough superlattices. A continuum model incorporating the effects of interface roughness indicates that diffuse scattering is dominant when y > 20 nm, and significant coherent transmission occurs when y < 20 nm.

High dimensionless figure-of-merit in nanostructured p-type bulk SiGe alloys, GIRI JOSHI, Boston College, HOHYUN LEE, Massachusetts Institute of Technology, XIAOWEI WANG, GOAHAU ZHU, YUCHENG LAN, DEZHI WANG, Boston College, BED POUDEL, GMZ Energy, Inc., MILDRED DRESSELHAUS, GANG CHEN, Massachusetts Institute of Technology, ZHIFENG REN, Boston College — Silicon Germanium (SiGe) alloys have been used for high temperature power generation in thermoelectric generators. Since their performance is related to dimensionless figure-of-merit (ZT), material scientists have focused their attention on possible improvements in ZT of SiGe alloys through an increase in power factor and decrease in thermal conductivity. We have been pursuing an approach of random nanostructures to reduce the thermal conductivity based on the understanding that the reduction of thermal conductivity is primarily responsible for ZT enhancement in superlattices. We have observed 100% improvement in ZT, compared to the state-of-the-art values, in p-type SiGe nanostructured bulk materials, which comes mainly from decrease in thermal conductivity due to the increase in phonon scattering by defects and grain boundaries in nanostructured. These bulk materials also possess superior mechanical properties making them more suitable for fabrication and integration into systems which were made by hot pressing of nanopowders prepared by using high energy ball milling.
1.39PM V35.00011 Nanotubular high thermoelectric figure-of-merit in n-type bulk SiGe alloys. XIAOWEI WANG, Boston College, HOHYUN LEE, Massachusetts Institute of Technology, GAOHUA ZHU, YUCHENG LAN, DEZHI WANG, Boston College, MILDRED DRESSELHAUS, GANG CHEN, Massachusetts Institute of Technology, ZHIFENG REN, Boston College, BOSTON COLLEGE TEAM, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION — Silicon germanium alloys (SiGe) have been the exclusive choice for radiotransfer thermoelectric generators (RTGs) because of its reliability and high operating temperatures. In this paper, by using mechanical alloying method, nano-sized phosphorous-doped (n-type) SiGe alloy powders were produced, followed by direct current induced hot press technique, bulk samples were obtained with ~100% density. The thermoelectric properties, including electrical conductivity, Seebeck coefficient, and thermal conductivity, were measured in the temperature range from 25 to 900 °C. A maximum ZT of around 1.3 at 900 °C was obtained under certain doping concentration and hot press conditions, mainly due to thermal conductivity reduction from nano-structured SiGe grains of 20 nm.

1Department of Mechanical Engineering/Department of Physics and Electrical Engineering

1:51PM V35.00012 Thermoelectric properties of n-type nano bulk Si. GAOHUA ZHU, Boston College, HOHYUN LEE, Massachusetts Institute of Technology, XIAOWEI WANG, GIRI JOSHI, YUCHENG LAN, JIAN YANG, DEZHI WANG, Boston College, MILDRED DRESSELHAUS, GANG CHEN, Massachusetts Institute of Technology, ZHIFENG REN, Boston College, DEPARTMENT OF PHYSICS, BOSTON COLLEGE TEAM, DEPARTMENT OF MECHANICAL ENGINEERING, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM, DEPARTMENT OF PHYSICS AND ELECTRICAL ENGINEERING, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM — Nano Si has been noticed as a promising substitute material for SiGe. We have observed a 150 to 350 % increase in ZT values in the heavily doped n-type nano Si over the single crystal Si, which mainly comes from the significantly lower thermal conductivity due to the nano size of grains achieved by mechanical alloying and hot press. The key to get higher ZT value is to optimize the doping concentration to achieve high power factor and avoid grain growth during hot-pressing to achieve nano particle size in the final bulk form. So far our research on nano bulk Si has shown promising ZT values close to 1, comparable to that of the traditional SiGe alloys. Silicon is lighter, more refractory, and has better thermal stability than Si_{1-x}Ge_{x} and also it is much cheaper than Ge. Pure Si may have advantage over SiGe alloy in mass application of power generation systems.

Thursday, March 13, 2008 11:15AM - 1:51PM -
Session V36 GIMS: Advances in Scanned Probe Microscopy IV: Optical and High Frequency Methods Morial Convention Center 228

11:15AM V36.00001 High-resolution element-selective microscopy using X-ray enhanced Scanning Tunneling Microscopy1, VOLKER ROSE, JOHN FREELAND, KENNETH GRAY, STEPHEN STREIFFER, MATTHIAS BODE, Argonne National Laboratory — Nanoscale structures are at the forefront of fundamental research as well as the keystone for whole new classes of potential applications. Proper understanding of these systems requires tools with both the ability to resolve the nanometer scale as well as provide detailed information about chemical, electronic and magnetic structure. Scanning probe microscopes achieve the requisite high spatial resolution; however, direct elemental determination is not easily accomplished. X-ray microscopes, on the other hand, provide elemental selectivity, but currently have spatial resolution only of tens of nanometers. We present a radically different concept that employs detection of local x-ray interactions utilizing a scanning probe that provides spatial resolution, and x-ray absorption directly yields chemical, electronic, and magnetic sensitivity. The achievement of nanometer spatial resolution with direct elemental selectivity will have a tremendous impact on our ability to probe and understand complex phenomena occurring in nanostuctures.

1This work was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-AC02-06CH11357. Corresponding author: vrose@anl.gov

11:27AM V36.00002 Scanning optical homodyne detection of high-frequency picoscale resonances in cantilever and tuning fork sensors1. J. C. RANDEL, G. ZELTZER, Stanford University, A. K. GUPTA, R. BASHIR, Purdue University, S.-H. SONG, H. C. MANOHARAN, Stanford University — Hybrid high-frequency sensors represent the next generation of scanned probe technology. In this work, higher harmonic modes in nanoscale silicon cantilevers and microscale quartz tuning forks are detected and characterized using a custom scanning optical homodyne interferometer. Capable of both mass and force sensing, these resonators exhibit high-frequency harmonic motion content with picometer-scale amplitudes detected in a 2.5 MHz bandwidth, driven by ambient thermal radiation. Quartz tuning forks additionally display both in-plane and out-of-plane harmonics. The first six electronically detected resonances are matched to optically detected and mapped fork eigenmodes. Mass sensing experiments utilizing higher tuning fork modes indicate greater than six times sensitivity enhancement over fundamental mode operation. (This work supported by NSF and ONR).


11:39AM V36.00003 Radio Frequency Scanning Tunneling Microscopy: Instrumentation and Applications UTKU KEMIKTARAK, Dept. of Physics, Boston University, Boston, MA 02215, TCHEFOR NDUKUM, KEITH C. SCHWAB, Dept. of Physics, Cornell University, Ithaca, NY 14853, KAMIL L. EKINCI, Dept. of Aerospace and Mechanical Eng., Boston University, Boston, MA 02215 — A severe limitation of the scanning tunneling microscope (STM) is its low temporal resolution, originating from the diminished high-frequency response of the tunnel current readout circuitry. In order to overcome this limitation, we have built a radio-frequency STM (RF-STM). Using this instrument, we can attain electronic bandwidths as high as 10 MHz by measuring the reflection from or transmission through the tunnel junction, which is embedded in a resonant inductor-capacitor (LC) circuit. This ~100-fold bandwidth improvement upon the state-of-the-art translates into fast surface topography as well as delicate measurements in mesoscopic electronics and mechanics. Broadband noise measurements across the tunnel junction using this radio-frequency-STM (RF-STM) have allowed us to perform nanoscale thermometry. Furthermore, we have detected high-frequency mechanical motion with a sensitivity approaching 15 fmHz^{-1/2}.
11:51AM V36.00004 Thermomechanical Noise Measurements of Very High Frequency (VHF) Nanomechanical Resonators¹, Carl Hart IV, Kamil Ekinçi, Aerospace and Mechanical Engineering, Boston University, Boston, MA — We have designed and built a near infrared (NIR) optical interferometer for ultra-sensitive displacement measurements on nanomechanical resonators. At moderate optical power levels, we are able to resolve the thermomechanical displacement fluctuations of stiff doubly-clamped beams with fundamental mode frequencies in the 100 MHz range. In a first set of noise measurements, we have determined the quality factors and resonant frequencies of the nanomechanical resonators under ambient atmospheric pressure at room temperature. We will compare these values to those extracted from driven resonance measurements and discuss sources of disagreement. Furthermore, we will discuss extraction of the local temperature of the nanomechanical resonators in order to assess the heating due to the optical probe.

¹This work was sponsored by the Department of the Air Force under Air Force Contract No. FA8721-05-C-0002 and NSF Award ECCS-0643178. The opinions, interpretations and conclusions belong to the authors and are not necessarily endorsed by the US Government.

12:03PM V36.00005 Development of an Evanescent Microwave Probe / Scanning Tunneling Microscope to study Localized Electron Spin Resonance, Christian Long, University of Maryland, Naoyuki Take-Toshi, National Institute of Advanced Industrial Science and Technology, Ichiro Takeuchi, University of Maryland, Haitao Yang, Intematix Corporation, Xiao-Dong Xiang, Intematix Corporation, University of Maryland Team, National Institute of Advanced Industrial Science and Technology Collaboration, Intematix Corporation Collaboration — We have constructed a microwave microscope with an integrated scanning tunneling microscope. In addition to the measurement of complex dielectric constant and conductivity we also perform atomic resolution scanning tunneling microscopy (STM). In this work the probe is operated in a magnetic field, which causes unpaired spins in the sample to precess at the Larmor frequency. When the magnetic field is such that the Larmor frequency of the spins in the sample matches the resonant frequency of the resonator, the transmission coefficient of the resonator (S12) is changed. We measure local ESR by measuring the variation in S12 as a function of magnetic field. In this report, we give an outline of the experimental setup and preliminary spin detection data for various spin radical molecules (one unpaired spin each) on an HPOG substrate (no unpaired spins). Supported by the W. M. Keck Foundation and NSF MRSEC (DMR 0520471).

12:15PM V36.00006 High Frequency Piezoresponse Force Microscopy in the 1-10 MHz Regime, Katayani Seal, Stephen Jesse, Brian Rodriguez, Arthur Baddorf, Sergei Kalinin, Oak Ridge National Laboratory — Imaging mechanisms in Piezoresponse Force Microscopy (PFM) in the high frequency regime above the first contact resonance are analyzed. High operation frequencies are expected to provide several advantages including (a) higher signal to noise ratios due to a larger number of oscillations per pixel time and increased separation from the 1/f noise corner (b) imaging at cantilever resonances with an associated increase in mechanical signal amplification (c) inertial stiffening of the cantilever that minimizes the non-local electrostatic force contribution to the signal and improves tip-surface contact. Furthermore, high frequency operation is an essential component of the PFM-based ferroelectric data storage systems, currently limited by the bandwidth of electromechanical detection (1-10 kHz). At the same time, operation at a high mode number can give rise to several problems, including the (a) response of averaging due to the finite size of the cantilever beam (b) loss of sensitivity if the tip-surface spring constant becomes smaller than the effective spring constant of the cantilever and (c) signal loss due to the bandwidth of the photodetector. Analytical expressions for these limits are considered. We analyze the operation mechanisms in PFM at high frequencies, and demonstrate high quality PFM imaging at 1-10 MHz. Prospects for imaging in the 10-100 MHz range are explored.

12:27PM V36.00007 Contrast sensitive imaging with a cantilever-based near-field microwave probe, Keiji Lai, Worasom Kundhikanjana, Michael Kelly, Zhi-Xun Shen, Geballe Laboratory for Advanced Materials, Stanford University — We have developed a procedure to systematically study the contrast mechanism of our cantilever-based near-field scanning microwave probes with separated excitation and sensing electrodes. Finite-element analysis was employed to model the small impedance change due to the tip-sample interaction. The near-field signal can then be calculated from the S-parameters of the matching network that routes the tip impedance to 50 Ohm feed lines. Using a common-mode cancellation scheme, the microwave electronics is sensitive down to 1aF capacitance change at our working frequencies near 1GHz. Experimental characterization of the microwave probes was performed on ion-implanted Si wafers and patterned semiconductor samples. Pure electrical or topographical signals, in qualitative agreement with simulation, can be obtained using different reflection modes of the probe. Our microscope also shows very high contrast due to conductivity variations of the sample, which can lead to potential applications of the technique.

¹The research is funded by the seed grant in Center of Probing the Nanoscale, Stanford University, NSF Grant No. PHY-0425897.

12:39PM V36.00008 STM and SNOM Type of Scanning Probe Microscopes in the Same Unit: Towards Electrical Modification and Optical Characterization at Nanoscale, Ilya Sychugov, NTB Basic Research Laboratories, Hiroo Omi, Tooru MuraShita, Yoshihiro Kobayashi — Optical and electrical properties of nanostructures can be addressed by radiation or electrical current as a probe. In general, a near-field type of electromagnetic interaction is necessary for an optical probe to enter nanoscale regime. However, a typical scanning near-field microscope utilizes a dielectric fiber tip as an aperture, which makes it unsuitable for electrical measurements. Here, in order to realize both electrical and optical probing at nanoscale, we have combined it with a scanning tunneling microscope (STM). An STM-luminescence (STML) instrument with a conductive and transparent tip, featuring about 40 nm spatial resolution, was reported previously. We have complemented it with a beamsplitter unit in a configuration typical for the fluorescent microscope. The excitation light is guided through a beamsplitter unit to the indium tin oxide (ITO) tip and the signal is collected via the same fiber transmission line in a spectroscopy mode or in a photon mapping regime. The influence of tip geometry on collection efficiency and spatial resolution as well as limitations of such an instrument are discussed. This approach may find its niche not only for combined electrical and optical measurements, but also for electrical modification with subsequent in situ optical probing.

12:51PM V36.00009 A Unique Probe for Tip Enhanced Raman Scattering and Shadow NSOM, Aaron Lewis, Hebrew University of Jerusalem, Hesham Taha, Rimma Dekhter, Galia Zinoviev, Galina Fish, Nanonics Imaging Ltd. — We present a unique atomic force microscope [AFM] probe for tip enhanced Raman scattering [TERS] and a new form of near-field microscopy, "Shadow Near-field Scanning Optical Microscopy". The probe consists of a single gold nanoparticle grown at the tip of a cantilevered nanopipette, exposed to the optical axis of an upright or inverted optical microscope. When these probes are used in combination with a Nanonics MV 2000 AFM/NSOM system, we show that a protocol for independent motion of the probe and the sample can produce enhancement or a shadow effect. Both of these effects are enhanced by the ability to affect different Raman spectra with the tip in & out of contact while independently scanning the sample. We analyzed Raman signals of a thin nanometric strained Si layer deposited on bulk Si and developed an understanding of optical mechanisms of enhancement, scattering and shadowing. Our results show different optical mechanisms occur as a result of tip & sample interactions, including TERS effect obtained by near-field interaction of the probe with the top layer of strained Si. Large enhancements of at least 4 orders of magnitude are seen and analyses of relative intensities of bulk and strained Si Raman peaks show an increase in light scattered by bulk or effective shadowing of the surface.
1:03PM V36.00010 Chemical Imaging of the Surface of Polymeric Nanostructures Using Aper- 
tureless Near-Field IR Microscopy
ZAHRA FAHKRAI, KERSTIN MUELLER, MELISSA PAULITE, XIUJUAN YANG, GILBERT C. 
WALKER, Department of Chemistry, University of Toronto, Toronto, ON, M5S 3H6, Canada — The 
chemical composition of the surfaces of thin films of polystyrene-poly (methyl methacrylate) (PS-PMMA) diblock copolymers is investigated using apertureless near-field IR microscopy. In this technique a tunable IR beam is scattered from an oscillating atomic force microscopy tip. The scattered light is enhanced using a reference signal with the same optical frequency (homodyne) or slightly shifted IR frequency (heterodyne) and detected after demodulation in order to eliminate the background scattering. Using this technique a lateral chemical imaging resolution of <20 nm is achievable. It is demonstrated that this technique can be successfully used to image the surface of PS-PMMA diblock copolymers. Another important result is that an increase in the IR absorption is observed in the PMMA rich domains with a wavenumber dependence that is consistent with the bulk absorption spectrum. The results indicate that even though a topography induced artifact can be observed, when homodyne detection technique is used, the chemical signature of the sample can be detected clearly. This technique can be further used in a variety of different systems to detect the surface structure of polymers or proteins.

1:15PM V36.00011 Scanning thermal microscopy with a fluorescent nanoprobe
BENJAMIN SAMSON, ELIKA SAIDI, LIONEL AIGOY, LPEM / CNRS, PETER LOW, LAAS / CNRS, BEMOJOON KIM, University of Tokyo, Japan, CHRISTIAN BERGAUD, LAAS / CNRS, MICHEL MORTIER, ENSCP / CNRS, LABORATOIRE PHOTONS ET MATIERE TEAM, LABORATOIRE D’ARCHITECTURE ET D’ANALYSE DES SYSTEMES TEAM, INSTITUTE OF INDUSTRIAL SCIENCE, CENTER FOR INTERNATIONAL RESEARCH ON MICROMECHATRONICS TEAM, LABORATOIRE DE CHIMIE DE LA MATIÈRE CONDENSÉE DE PARIS TEAM — We have developed a scanning thermal microscope that uses a fluorescent particle settled at the extremity of an atomic force microscope tip as a nanoscale temperature sensor. When a temperature change occurs, a modification of fluorescence is detectable, enabling to perform thermal images and to determine the local temperature. We will describe the technique in details and present some thermal images on submicron sized nickel nanoheaters heated by an electrical current. We will show that this apparatus works in both DC and AC regimes, in a low frequency range whose upper limit is around the kilohertz. By performing tip approach/retraction curves on a heated wire, we will describe the different thermal transfer mechanisms between the surface and the fluorescent probe.

1:27PM V36.00012 A versatile technique for fabrication of SiC SPM probes
JOEL THERRIEN, DANIEL SCHMIDT, SHEETAL BARROT, BHAVIN PATEL, U. Massachusetts-Lowell — To date SPM probes have largely been fabricated via methods borrowed from the semiconductor industry for fabricating Micro Electro Mechanical Systems. Although these techniques have enabled SPM to see widespread use, the processes put significant limitations on what structures can be made. We report our progress on fabricating SPM cantilevers composed of Silicon Carbide using polymer molding techniques. A pre-ceramic polymer is molded into the desired probe shape and then converted to SiC via pyrolisys. We will also report on progress in using photo-sterolithography for fabrication of even more complex geometries. In addition to opening up a much larger set of probe structures, the use of SiC leads to improved wear resistance of the resulting probes. Among the potential applications, this method enables the fabrication of low spring constant, high resonant frequency cantilevers via cross sectional geometries not accessible to standard fabrication techniques. Such probes are required for high speed tapping and non-contact imaging.

1Seed funding provided by the NSF supported Center for High-rate Nanomanufacturing at UML

1:39PM V36.00013 In-situ broadband microwave calibrations and measurements using cryo-
genic probe stations
JEFFREY LINDEMUTH, SCOTT YANO, Lake Shore Cryotronics — Until recently, calibration of microwave measurements in cryogenic environments required custom fixtures [1,2]. These fixtures were necessary to accommodate the limited space in typical “down bore” cryostat designs. The typical three measurements (through, short, load, for example) required removing the fixtures from the cryostat three times before loading the sample of interest. We will show that with a 4-probe cryogenic probe station it is possible to simultaneously load a commercially available calibration test strip and the measurement sample. We will demonstrate calibration of the complete S matrix of the microwave network analyzer at each temperature followed by measurement of the sample. In addition, the temperature-dependent effects of the calibration can be determined. We will show short term and long term calibration stability.
[2] Broadband microwave spectroscopy in Corbino geometry for temperatures down to 1.7 K

Thursday, March 13, 2008 11:15AM - 2:03PM –
Session V37 FlAP: QHE and FQHE Morial Convention Center 229

11:15AM V37.00001 Optical Studies of Quantum Phases with Filling Factors 2 ≤ ν ≤3 in 
the Second Landau Level
TREVOR DAVID RHONE, JUN YAN, Columbia University, YANN GALLAIS, Université Paris7, ARON PINCZUK, Columbia University, LOREN PFEIFFER, KEN WEST, Bell labs, Alcatel-Lucent — We report low temperature inelastic light scattering and optical recombination measurements of quantum phases in the second Landau level of 2D electron systems. We focus on states with filling factors 2 ≤ ν < 3. An ultra high mobility, high density GaAs quantum well (240nm) is probed at low temperature (42mK – 1.2K). Low energy spin excitations are studied by resonant inelastic light scattering. We confirm the existence of a ferromagnetic state at ν = 3 by the observation of a well defined long wavelength spin wave mode at the Zeeman energy. Surprisingly, the ferromagnetic spin wave collapses at filling factors slightly away from ν = 3. While this behavior may be a signal of the disappearance of ferromagnetic order in the second Landau level, experiments in progress may offer deeper insights on fundamental interactions and quantum phases in the second Landau level.

1Supported by NSF and DOE

11:27AM V37.00002 Investigations of possible Landau level anticrossings in p-type (110) GaAs 
square wells
NEBILE ISIK, SIF. ROTH, M. BICHLER, A. FONTCUBERTA I MORRAL, G. ABSTREITER, Tech. Univ. Muenchen, M. GRAYSON, Northwestern University — In p-type (110) quantum wells, a single anomalous magnetoresistance peak is observed within the lowest Landau level (ν = 1) of a two-dimensional hole system when the confinement is a triangular potential well [1]. This peak is interpreted as the transport signature of a ± 3/2 spin-reversal level-anticrossing in the lowest Landau level. In recently fabricated 400 Åwide square quantum wells, we observe peaks within several Landau levels, for example, at both ν = 1 and ν = 2. The peak positions in magnetic field B are observed shift with top gate bias and the peak magnitudes are observed to increase with increasing temperature. At a critical top gate bias, however, both original peaks disappear, just as new features appear at higher fields within both the ν = 1 and ν = 2 minima. Dependence of feature position on front and back gate bias will be shown, and temperature dependences will be studied in terms of activated energy gaps. The cause of these peaks will be discussed in terms of possible multiple Landau level anticrossings.

1Supported by DFG Grant GR-2618/1-1
11:39AM V37.00003 Current Instability Induced by Negative Differential Conductivity in the Quantum Hall Regime1, KUAN TING LIN, YULING TSAI, YIPING LIN, J. C. CHEN, Dep. of Physics, National Tsing Hua University, Hsinchu, Taiwan, T.UEDA, S. KOMIYAMA, Dep. of Basic Science, University of Tokyo, Meguro-ku, Tokyo, Japan — We report a new kind of nonlinear effect at \( \nu = 2 \) Hall plateau in a two-dimensional electron gas system formed on a GaAs/AlGaAs heterostructure. Within the temperature \( 16 \, K \leq T \leq 28 \, K \), the current shows discernible zig-zag feature as the applied dc electric field increases beyond a critical value. Such an unstable feature is not only reproducible but also exhibits hysteresis as changing the sweeping direction of the electric field. We identify this current instability as the occurrence of the negative differential conductivity induced by the electric field. Physical origin of the nonlinearities will be presented and discussed.

1Supported by National Science Council (Taiwan)

11:51AM V37.00004 New Observations in the \( N \geq 1 \) Landau Levels of Wide GaAs Quantum Wells, D.R. LUIHMANN, Princeton University, W. PAN, Sandia National Laboratories, D.C. TSUI, Princeton University, L.N. PFIEFFER, K.W. BALDWIN, K.W. WEST, Bell Laboratories — We have studied a series of high-quality wide GaAs/AlGaAs quantum wells at various tilt angles \((\theta)\) with respect to magnetic field. Several interesting observations have been made when the Landau level index is \( N \geq 1 \). The quantum Hall states corresponding to total odd filling factors are seen to be reentrant with increasing \( \theta \), i.e. they disappear and reemerge as \( \theta \) is increased. This observation can be explained by considering oscillations in the tunneling amplitude with increasing \( \theta \). As \( \theta \) is increased further, anisotropy emerges at values of half filling. This is particularly visible in the \( N = 1 \) Landau level at total filling factors \( \nu = 9/2 \) and \( 11/2 \). For even larger values of \( \theta \), anisotropy develops at \( \nu = 5 \) followed by \( \nu = 7 \). We will discuss how each of these observations are effected by quantum well width and also in the context of previous theoretical and experimental results.

12:03PM V37.00005 Edge state tunneling in a point contact at filling fraction \( \nu = 5/2 \), IULIANA P. RADU, MIT, J.B. MILLER, C.R. DILLARD, C.M. MARCUS, Harvard University, M.A. KASTNER, MIT, L.N. PFIEFFER, K.W. WEST, Bell Labs, Alcatel-Lucent — We investigate low temperature transport properties of quantum point contacts (QPCs) fabricated in a GaAs/AlGaAs 2-dimensional electron gas (2-DEG) with mobility \( 2000 \, \text{m}^2/\text{Vs} \) in a perpendicular magnetic field. The 2-DEG exhibits fractional quantum Hall effect, including a well-quantized plateau at \( \nu = 5/2 \). We study the temperature and DC current bias dependence of the transport through the QPC at \( \nu = 5/2 \) while preserving the same filling number in both the QPC and the bulk of the sample. We compare our results to theoretical predictions for quasi-particle tunneling in the weak coupling regime, and extract the quasi-particle charge and the strength of the Coulomb interaction, as reflected by the Luttinger liquid parameter \( g \). This work was partially supported by ARO (W911NF-05-1-0062), by the NSEC program of NSF (PHY-0117795), by NSF (DMR-0353209) at MIT and by Project Q of Microsoft Corporation at Harvard University.

12:15PM V37.00006 Stripes and Bubbles in the \( N=2 \) Landau Level: A DMRG Study, BARRY FRIEDMAN, LAUREN ROD, CANDICE WITHROW, Department of Physics, Sam Houston State University — The phase diagram of the \( N=2 \) Landau level has been reexamined using the density matrix renormalization group (dmrg). Very good agreement at filling factor \( 18/42 \) has been attained with previous dmrg calculations of Shibata and Yoshioka by using 200 states in the blocks. Near \( 1/2 \) filling, we have studied whether the ground state is an anisotropic crystal, suggested by some mean field approaches, or a stripe state, as suggested by other mean field approaches and previous dmrg results. Previous dmrg calculations, i.e. Shibata and Yoshioka, have placed the phase diagram between stripes and bubbles at a filling factor slightly less then \( 4 \) by looking at the projected pair correlation function at the special lines \( x=0 \) and \( y=0 \). We reexamine this boundary by studying the Fourier transform of the projected pair correlation.

12:27PM V37.00007 Interactions and Landau level mixing at large half odd-integer filling, PETER SMITH, MALCOLM KENNETT, Department of Physics, Simon Fraser University — Recent transport experiments on two-dimensional hole systems (2DHs) in a strong perpendicular magnetic field show variations in the anisotropy of resistivity at half odd-integer filling fractions \( \nu = 7/2 \), \( 9/2 \), and \( 11/2 \) that differ from those seen in two-dimensional electron systems. It has been suggested that spin-orbit coupling in 2DHs leads to these unusual transport properties, as it gives rise to Landau level mixing. We consider the general problem of interacting fermions subject to a perpendicular magnetic field with Landau level mixing in the limit of large Landau levels, and discuss the effect of Landau level mixing on charge-density wave formation in comparison to the single Landau level case. We study the case of spin-orbit induced mixing in detail, and discuss implications for experiments.


12:39PM V37.00008 Interaction effects in transport through an electronic Mach-Zehnder interferometer, VITALY GOLOVACH, FLORIAN MARQUARDT, Department of Physics, Arnold-Sommerfeld-Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-University Munich, Germany — We study theoretically transport through an electronic Mach-Zehnder interferometer in the presence of Coulomb interaction inside the interferometer, using a discrete wave-packet model. We find that the mutual capacitance between the arms of the interferometer leads to a suppression of the visibility of the Aharonov-Bohm oscillations at a large source-drain bias \( \Delta \mu \gg h \nu_{\text{c}} / L \), where \( L \) is the length of the arms and \( \nu_{\text{c}} \) is the electron drift speed. Our numerical simulations indicate that the visibility of the Aharonov-Bohm oscillations is a non-analytic function of the mutual capacitance strength, in the limit \( \Delta \mu \rightarrow \infty \).

12:51PM V37.00009 Universal Periods in Quantum Hall Droplets1, GREGORY A. FIETE, GIL REFAEL, California Institute of Technology, MATTHEW P. A. FISHER, Microsoft Station Q, UCSB — Using the hierarchy picture of the fractional quantum Hall effect, we study the the ground state periodicity of a finite size quantum Hall droplet in a quantum Hall fluid of a different filling factor. The droplet edge charge is periodically modulated with flux through the droplet and will lead to a periodic variation in the conductance of a nearby point contact, such as occurs in some quantum Hall interferometers. Our model is consistent with experiment and predicts that superperiods can be observed in geometries where no interfering trajectories occur. The model may also provide an experimentally feasible method of detecting elusive neutral modes and otherwise obtaining information about the microscopic edge structure in fractional quantum Hall states.

1:03PM V37.00010 Variational Monte Carlo study of the nematic state at half-filled Landau level of the two dimensional electron gas, QUOC DOAN, Florida State University, EFSTRATIOS MANOUSAKIS, Florida State University, Center for Materials Research and Technology — The nematic state of 2DEG at half-filled Landau level (LL) is investigated using the variational Monte Carlo method. The wave function used has Jastrow correlations of the form $\prod_{i<j}(z_i - z_j)^2$ and a Slater determinant having an elliptical Fermi sea. We use the unprojected version of the wave function and apply the Monte Carlo (MC) method to calculate the pair distribution functions and the optimum energies. We compare optimum energies of the nematic state obtained by MC and Fermi hypernetted chain (FHNC/0) approximation with the optimum energies of the stripe ordered state obtained by Hartree-Fock. We find that both FHNC/0 and MC suggest that the nematic state may be energetically favorable as compared to the stripe ordered state at 2nd LL. We have obtained the exact projection of the above mentioned wavefunction of the nematic phase onto the lowest LL. We are in the process of comparing the results obtained with the exact wavefunction on small size systems to those obtained without the projection.

1:15PM V37.00011 Anisotropy in two-dimensional electronic quantum Hall systems at half filling of valence Landau levels, ORION CIFTJA, Department of Physics, Prairie View A&M University, Prairie View, TX 77446, USA, CARLOS WEXLER, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA — A recent experimental discovery in the quantum Hall regime has been the observation of very strong magneto-transport anisotropies at certain low values of magnetic field below a critical temperature of about 100 mK. While the origin of such anisotropy is yet unknown, we explain the emergence of such anisotropies in terms of electronic liquid crystalline states with broken rotational symmetry. We investigate the stability of liquid crystalline phases with nematic order at half filling of the valence Landau level. Quantum Monte Carlo simulations indicate that while isotropic states are stable in the lowest and first excited Landau level, there are regions of instability towards liquid crystalline states in higher Landau levels. A possible connection of the recently discovered magneto-transport anisotropy in low magnetic fields and these liquid crystalline states is discussed.

1:27PM V37.00012 Quantum Hall hierarchy wave functions from conformal field theory, SUSANNE VIEFERS, University of Oslo, Norway, EMIL BERGHLOTZ, HANS HANSSON, MARIA HERMANNS, ANDERS KARLHEDE, Stockholm University — It has long been known that Laughlin’s wave functions, describing the fractional quantum Hall effect at filling fraction $\nu = 1/(2l+1)$, can be obtained as correlation functions in conformal field theory. We show how to generalize this approach to construct explicit trial wave functions for all states in the quantum Hall hierarchy corresponding to quasi particle (as opposed to quasihole) condensates, including the recently observed state at $\nu = 4/11$. At the filling fractions $\nu = n/(2np+1)$ this construction exactly reproduces Jain’s composite fermion wave functions. An explicit connection is made to Wen’s topological classification of FQH states.

1:39PM V37.00013 FQHE-the soluble limit and beyond, MARIA HERMANNS, EMIL J. BERGHOLTZ, THORS HANS HANSSON, ANDERS KARLHEDE, Stockholm University, JUHA SUORSA, Helsinki University of Technology — We consider the quantum Hall system in the torus geometry. In the limit where the torus becomes thin, the problem is exactly soluble and the hierarchy of quantum Hall states is manifest. Explicit wave functions for a large set of them are constructed with help of conformal field theory. This construction provides a continuation from the exactly soluble limit to the experimental regime. Numerical results on 4/11 supports this picture.

1:51PM V37.00014 The Quantum Hall Effect in Spin Quartets in Graphene, KEISHAV SHRIVASTAVA, University of Malaya — Using the non-relativistic Schroedinger equation, we find that for $(1/2)g=(1/2)\pm 1$ gives zero charge for negative sign and one charge for positive sign. This explains the conductivity at $i=0$ and $1$. For $s=3/2, (1/2)g=2$ for positive sign and hence $g=4$. The substitution in the series, $-(5/2)(g\mu_B H), -(3/2)(g\mu_B H), -(1/2)(g\mu_B H), +(1/2)(g\mu_B H), +(3/2)(g\mu_B H), +(5/2)(g\mu_B H), . . . . , etc., g=4 gives, -10, -6, -2, +2, +6, +10, etc. This series is the same as observed in the experimental data of quantum Hall effect in graphene. When we take $n=2$ in the flux quantization, i.e., $2(hc/e)$, we generate the plateaus at $i=0$ and 1. For $s=3/2$ gives zero charge for negative sign and one charge for positive sign. This explains the conductivity at $i=0$ and $1$. For $s=3/2, (1/2)g=2$ for positive sign and hence $g=4$. The substitution in the series, $-(5/2)(g\mu_B H), -(3/2)(g\mu_B H), -(1/2)(g\mu_B H), +(1/2)(g\mu_B H), +(3/2)(g\mu_B H), +(5/2)(g\mu_B H), . . . . , etc., g=4 gives, -10, -6, -2, +2, +6, +10, etc. This series is the same as obtained in the experimental data of quantum Hall effect in graphene. When we take $n=2$ in the flux quantization, i.e., $2(hc/e)$, we generate the plateaus at $\pm 4$. Thus the plateaus can occur at 0, 1, 4 and at 2, 6, 10, 14, . . . . etc. Thus the quantum Hall effect in graphene is understood by means of non-relativistic theory. The fractions such as $1/3$ or integers such as $0,1,4, . . . . 2,6,10,14, . . .$ multiply the charge and hence describe the “effective charge” of the quasiparticles. This means that there is “spin-charge locking”.


Thursday, March 13, 2008 11:15AM - 2:15PM — Session V38 DCMP: Focus Session: Multiferroics and Multiferroic Composites Morial Convention Center 230

11:15AM V38.00001 In pursuit of strongly coupled multiferroic oxides, CRAIG FENNIE, Argonne National Lab — The rational design of new materials with emergent properties is a riveting challenge today in materials physics. It begins with understanding a mechanism to control the interplay between diverse microscopic degrees of freedom in order to create targeted macroscopic phenomena and ends with the discovery or design of new material realizations. When combined with first-principles density-functional theory, this approach provides an efficient strategy to survey the vast space of possible materials to target for synthesis. In this talk I will discuss our recently proposed strategies to identify new multiferroic oxides in which magnetism not only coexists with but also is strongly coupled to ferroelectricity. In one case the interplay of spins, optical phonons, and strain leads to a competition between different ordered states producing a colossal magnetoelectric effect. In a second case, a ferroelectric distortion can be designed to induce weak-ferromagnetism facilitating the electric-field control of a switchable magnetization. We also present first-principles density-functional calculations for several potential realizations.

11:51AM V38.00002 Growth and characterization of YMnO$_3$ nanocrystalline prisms, E. RAMOS-MOORE, Facultad de Fisica, Pontificia Universidad Catolica de Chile, CAMERON KEENAN, SANDEEP CHANDRIL, Department of Physics, West Virginia University, A. L. CABRERA, Facultad de Fisica, Pontificia Universidad Catolica de Chile, THOMAS H. MYERS, Department of Physics, West Virginia University, DAVID LEDERMAN, Department of Physics, West Virginia University, WEST VIRGINIA UNIVERSITY COLLABORATION, PONTIFICIA UNIVERSIDAD CATOLICA DE CHILE COLLABORATION — YMnO$_3$ epitaxial self-assembled nanoprisms were grown on GaN by molecular beam epitaxy. The prisms formed suddenly after 6 unit cells during Stranski-Krastanow epitaxial growth at 850 °C, with sizes ranging from 20 nm to 60 nm in height and 50 nm to 260 nm in lateral dimensions. They were characterized via energy dispersive analysis of x-rays (EDAX) mapping and x-ray diffraction and reflectivity. EDAX line scans across the prisms showed that the prisms were composed of YMnO$_3$. X-ray diffraction showed a 2.2% strain along the growth direction and a 1.6% compression in the plane when compared to bulk lattice parameters.

This work was funded by ONR (Grant N00014-02-1-0974), the AFOSR (MURI grant F49620-03-1-0330), and NSF (CIAM-DMR grant 0502825) at WVU and by FONDECYT (grant 1060634) at PUC.
12:03PM V38.00003 Properties of YMnO₃ Self-assembled Nanocrystalline Prisms on GaN¹, CAMERON KEENAN, SANDEEP CHANDRIL, THOMAS H. MYERS, DAVID LEDERMAN, Dept of Physics, West Virginia University, ESTEBAN RAMOS-MOORE, ALEJANDRO L. CABRERA, Facultad de Fisica, Pontificia Universidad Catolica de Chile — The high-temperature (850 °C) molecular beam epitaxy deposition of YMnO₃ on HVPE GaN(0001) resulted in the formation of spontaneous ferroelectric domains. Their dimensions ranged from 20 nm to 60 nm in thickness and 50 nm to 500 nm in lateral size. The local dielectric properties of the sample were investigated using scanning surface potential microscopy (SSPM). Raman remanent hysteresis loops were used to compare the switching properties of the samples and underlying film. A larger remanence was observed for the prisms, most probably due to the lack of surrounding film areas that would clamp the ferroelectric response. As a result, the remanent polarization increased roughly linearly with increasing prism surface area.

¹This work was funded by ONR (Grant N00014-02-1-0974), the AFOSR (MURI grant F49620-03-1-0330), and NSF (CIAM-DMR grant 0502825) at WVU and by FONDECYT (grant 1060634) at PUC.

12:15PM V38.00004 Epitaxial growth and electrical properties of perovskite HoMnO₃ thin films, DAISUKE KAN, M. MURAKAMI, Department of Materials Science and Engineering, University of Maryland, W. YU, R.L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, S.W. CHEONG, Department of Physics and Astronomy, Rutgers University, I. TAKEUCHI, Department of Materials Science and Engineering, University of Maryland — Recently, it was predicted that orthorhombic HoMnO₃ would exhibit relatively large polarization (of the order of μC/cm²) due to the existence of a ferroelectric order in the E₃ type magnetic structure [1]. We have fabricated perovskite HoMnO₃ thin films on SrTiO₃ (001) substrates by pulsed laser deposition. X-ray 2θ scan shows only indicating that there are no secondary phases. The reciprocal space mapping around the SrTiO₃ (103) Bragg reflection and the φ scan of the HoMnO₃ (103) peak reveals the tetragonal symmetry of the films and the epitaxial relationship, [100]HoMnO₃ // [100]SrTiO₃ and [001]HoMnO₃ // [001]SrTiO₃, confirming that the film has the perovskite structure and not the tetragonal one. The films show good insulating properties at low temperatures. We will present electrical properties of the films including results of FUND measurements in applied magnetic field below the Neel temperature. This work is supported by NSF MRSEC, ARO, and the W. M. Keck Foundation.

12:27PM V38.00005 Magnetic ground state of PbVO₃ and origin of the large tetragonal distortion, KENGO OKA, IKUYA YAMADA, MASAKI AZUMA, MIKIO TAKANO, YUICHI SHIMAKAWA, Inst. Chem. Res., Kyoto Univ., SOSHI TAKESHITA, KOHKI H. SATOH, AKIHITO KODA, RYOSUKE KADONO, Inst. Mater. Sc. & KEK, HIROSHI KOJITANI, MASAKI AOKI, Gakushin Univ. — Magnetic property of PbTiO₃-type perovskite PbVO₃ with a large tetragonal distortion (c/a = 1.23)¹ was investigated. Long-range antiferromagnetic ordering with T_N = 45 K was found by a μSR measurement. Magnetic susceptibility of multi domain crystal showed a broad maximum centered at 180 K indicated the 2-dimensional nature in magnetism. This is consistent with the d_{xy} orbital ordering predicted by the band calculation.² We propose a mechanism that the pyramidal coordination with a short vanadium-apical oxygen bond is stabilized to lift the orbital degeneracy in this d² system. Accordingly, PbMnO₃ (Mn⁴⁺, d⁰) newly stabilized at 15 GPa has a pseudo cubic structure like PbCrO₃. This scenario explains the pressure induced tetragonal to cubic, insulator to metal transition³ of PbVO₃ and similar large tetragonal distortion of BiCoO₃. [1] A. Belik, et al., Chem. Mater. 18 (2006) 798. [2] Y. Uratani, et al., Jpn. J. Appl. Phys., 44 (2005) 7130.

12:39PM V38.00006 A one-cent room-temperature magnetoelectric sensor, CASEY ISRAEL, NEIL MATHUR, Department of Materials Science, University of Cambridge, JAMES SCOTT, Department of Earth Sciences, University of Cambridge — The replacement of silver-palladium with nickel as an electrode material might be adopted as cheap magnetic-field sensors that do not require an electrical power source.

12:51PM V38.00007 Inversion symmetry controlled multiferroic response in an Ising Chain Magnet, YOUNJUNG JO, SEONGSU LEE, HEE TAEK YI, SANGWOOK CHEONG, LUIS BALICAS, NATIONAL HIGH MAGNETIC FIELD LABORATORY TEAM, RUTGERS CENTER FOR EMERGING MATERIALS AND DEPARTMENT OF PHYSICS & ASTRONOMY TEAM — Recently, Choi et al. [1] discovered that ferroelectricity in the Ising chain magnet results from inversion symmetry breaking due to the formation of an alternating ionic order of two different ions leading to an up-up-down-down spin configuration. Here we report the observation of drastic changes in the multiferroic character as a function of temperature variation and through applied magnetic fields. In order to understand the origin of this inter-relationship, we have performed comprehensive characterization experiments on the multiferroic compound, including measurements of dielectric constant, polarization, specific heat, magnetic susceptibility, and resonant x-ray scattering as functions of temperature and applied magnetic field.

1:03PM V38.00008 Inter-relationship among magnetization, polarization and magnetic wave vector in multiferroic spinel CoCr₂O₄, YOUNG JAI CHOI, JUN OKAMOTO, DI-JING HUANG, KUO SHENG CHAO, HONG-JI LIN, CHIEN-TE CHEN, MICHEL VAN VEEENDAAL, THOMAS A. KAPLAN, SANGWOOK CHEONG — It has been known that the spinel CoCr₂O₄ is a multiferroic with conical spiral magnetic order characterized by three physical parameters: magnetization (M), polarization (P) and magnetic modulation vector (Q). We have found that these observables have a close inter-relationship in the multiferroic state and their inter-relationship changes in a methodical manner upon temperature variation and through applied magnetic fields. In order to understand the origin of this inter-relationship, we have performed comprehensive characterization experiments on the multiferroic compound, including measurements of dielectric constant, polarization, specific heat, magnetic susceptibility, and resonant x-ray scattering as functions of temperature and applied magnetic field.

1:15PM V38.00009 Structural and Dielectric Properties of CoFe₂O₄-Ba₀.90La₀.067Ti₀.91Zr₀.09O₃ Composite thin films, EDUARDO DELGADO, Universidad del Valle, CARLOS OSTOS, Universidad Nacional, MARIA MARTINEZ, LOURDES MESTRES, Universidad de Castilla-Leon, DAVID LEDERMAN, West Virginia University, PEDRO PRIETO, Centro de Excelencia en Nuevos Materiales — CoFe₂O₄-Ba₀.90La₀.067Ti₀.91Zr₀.09O₃(CFO-BLZT) composite thin films were grown via RF oxygen magnetron sputtering from a CFO-BLZT mixed target on electrically-conducting single-crystal Nb-doped SrTiO₃ (100) substrates at 1033 K. From scanning electron microscopy coupled with energy dispersive analysis of x-rays we determined that the CFO and BLZT were phase separated. X-ray photoemission spectroscopy showed that the TiO₂ octahedron in the perovskite structure was modified by the lanthanide incorporation. The dielectric characterization showed that the samples were ferroelectric at room temperature. The ferroelectric hysteresis loops measured as a function of magnetic field showed that these samples are multiferroic.
1:27PM V38.00010 Studies of Magnetoelectric properties in (1-x)Pb(Fe$_{2/3}$W$_{1/3}$)$_2$O$_3$-xPbTiO$_3$ solid solutions thin films, ASHOK KUMAR, University of Puerto Rico, RAM KATIYAR, University of Puerto Rico — We have fabricated (1-x)Pb(Fe$_{2/3}$W$_{1/3}$)$_2$O$_3$-xPbTiO$_3$ (PFWT) (x=0.50) thin films on Pt/Si substrates using sol-gel technique. The XRD patterns revealed a single-phase nature of the compound. The microstructure and surface morphology were investigated using SEM and AFM techniques that indicated good homogeneity and had surface roughness of 10-15 nm with particle size of ~ 30-50 nm. The dielectric relaxation studies in these films were carried out measured in the temperature range of 100K-650K and the frequency range of 100Hz-1MHz. Raman and dielectric data indicate that the crystal structure changes from tetragonal to cubic i.e. a ferroelectric phase transition at 575K. The dielectric properties of PFWT thin films were studied in the temperature range 80-600 K over a wide range of frequencies. The slope of the reciprocal of the dielectric constant is 2:1, matched well with the simplest Landau free energy model and it indicates continuous second order displacive ferroelectric phase transition. The polarization hysteresis curve at room temperature illustrated a ferroelectric nature. The detailed of magnetc and magnetoelectric properties with of PFWT will be discussed.

1:39PM V38.00011 Magnetoelectric Effects in hexagonal ferrite-PZT bilayers, V.M. MATHE, G. SRINIVASAN — Materials Science and Engineering, Penn State University — Fe (001) films have been epitaxially grown on ferroelectric Co$_3$Z and Zn$_2$Y are well known hexagonal ferrites with easy plane or uniaxial anisotropies. PZT has high piezoelectric coefficient. This study is on samples with Co$_3$Z or Zn$_2$Y as a magnetostrictive layer and PZT as a piezoelectric layer to form magnetoelectric bilayers. Low frequency (100 Hz) ME coefficient was measured over 0-17 kOe for various orientations of bilayers in a plane parallel to ac and bias magnetic fields. We measured a strong dependence of the ME voltage coefficients on magnitude and orientation of the bias field. The data are compared with theory.

2:03PM V38.00013 Dynamic observation of magnetoelectric coupling effect using magnetic force microscopy and Lorentz TEM, SUNG HWAN LIM, TODD BRINTLINGER, DAIJUKE KAN, YI QI, JOHN CUMINGS, ICHIRO TAKEUCHI, LOURDES SALAMANCA-RIBA — Magnetoelctric Effects in hexagonal ferrite-PZT bilayers, Materials Science and Engineering, Penn State University — Fe (001) films (30 nm) have been epitaxially grown on ferroelectric Co$_3$Z/SrTiO$_3$(001) to study the interaction between the multiferroic components. We report the magnetic properties as a precursor to a full investigation of the multiferroic interactions. Ferromagnetic resonance measurements were carried out at 36 GHz cavity and variable frequency microstrip resonators. Four-fold anisotropy is present in these Fe (001) films with energy density $\sim$1.3x10$^6$ erg/cm$^3$, consistent with bulk Fe values and indicating high quality Fe grown on the ferroelectric. Also present is a small, additional resonance peak, with large out-of-plane uniaxial anisotropy ($\sim$0.75$^2$(20$^2$)) attributed to strained Fe at the interface, although structural data shows the majority of the film is relaxed. This interfacial Fe will likely provide the desired coupling between the ferromagnetic and ferroelectric components in the system. Frequency/fiel in-plane dispersion curves further confirm the high quality of the Fe films in these samples.

This work was supported by NSF MRSEC DMR 0520471, ARO 28D1083899, ONR-MURI N000140610930.


11:15AM V39.00001 Anisotropic power-laws in sheared amorphous solids, CRAIG MALONEY, CMU — Dept. of Civil and Environmental Engineering, MARK ROBBINS, Johns Hopkins; Dept. of Physics and Astronomy — The local deformation of two-dimensional Lennard-Jones glasses under imposed shear strain is studied via computer simulations. Spatial correlations in the strain field are highly anisotropic and show apparent power-law behavior with a dramatic angular dependence of the effective scaling exponent. The strongest correlations are for wavevectors roughly perpendicular to the line of maximum resolved shear stress with systematic deviations from this which can be understood in terms of a Mohr-Coulomb effect. These results shed light on the nature of the so-called Jamming transition, supporting the notion that the dense steady flowing state is effectively critical in the slow-driving limit, and provide important, testable predictions for experiments on sheared amorphous materials such as bubble rafts, foams, emulsions, granular packings, etc., which can directly access the particle displacements.

11:27AM V39.00002 Apparent critical scaling for a steady-state sheared glass, THOMAS HAXTON, ANDREA LIU, University of Pennsylvania — We conducted simulations of a two-dimensional model glass at nonzero temperature under steady-state shear, and calculated the shear stress and shear viscosity as a function of temperature, shear rate and density. Over a dynamic range of two to three decades, we find excellent collapse of the data using critical scaling of the shear viscosity as a function of the distance from the jamming surface in the parameter space spanned by temperature, shear stress, and density. The shear viscosity can be rescaled to collapse onto a master function of the rescaled stress, where the scale factors are powers of the displacement in parameter space from the critical jamming surface. The master function separates into two branches, a high-temperature or low-density branch that approaches a finite rescaled viscosity at low stress, and a low-temperature or high-density branch that appears to diverge at a finite value of the rescaled stress. These results are consistent with those of Olsson and Teitel[1], who found scaling collapse near the zero-temperature, zero shear-stress jamming transition. We compare our results to mode-coupling calculations of sheared systems. [1] P. Olsson and S. Teitel, Phys. Rev. Lett. 99, 178001 (2007).

This work was supported by NSF-DMR-0605044.

1:51PM V38.00012 Magnetic properties in multiferroic Fe/BaTiO$_3$/SrTiO$_3$(001), M. PECHAN, C. YU — Physics, Miami University, S. SRIVASTAVA, C. PALMSTROM — Chemical Engineering & Materials Science, University of Minnesota, M. BIEGALSKI, C. BROOKS, D. SCHLOM — Materials Science and Engineering, Penn State University — Fe (001) films (30 nm) have been epitaxially grown on ferroelectric BaTiO$_3$/SrTiO$_3$(001) to study the interaction between the multiferroic components. We report the magnetic properties as a precursor to a full investigation of the multiferroic interactions. Ferromagnetic resonance measurements were carried out at 36 GHz cavity and variable frequency microstrip resonators. Four-fold anisotropy is present in these Fe (001) films with energy density $\sim$1.3x10$^6$ erg/cm$^3$, consistent with bulk Fe values and indicating high quality Fe grown on the ferroelectric. Also present is a small, additional resonance peak, with large out-of-plane uniaxial anisotropy ($\sim$0.75$^2$(20$^2$)) attributed to strained Fe at the interface, although structural data shows the majority of the film is relaxed. This interfacial Fe will likely provide the desired coupling between the ferromagnetic and ferroelectric components in the system. Frequency/fiel in-plane dispersion curves further confirm the high quality of the Fe films in these samples.

Acknowledgement: supported by U.S. DoE at MU and U.S ONR-MURI at UM.
an atomic description of the viscosity of a supercooled liquid capturing the highly non-Arrhenius temperature variation for which no previous calculation has been given. A temperature dependent activation energy for structural relaxation is derived by mapping the potential energy surface and extracting saddle-point configurations and associated atomic coordinates. This essential information is combined with the temperature variation of an effective local energy minimum (inherent structure) to describe shear relaxation by thermal activation. For a binary Lennard-Jones model the calculated viscosity shows a characteristic crossover from strong (Arrhenius) to fragile (highly non-Arrhenius) behavior upon appreciable undercooling; followed by a second crossover from fragile back to strong behavior on approaching the glass transition temperature, both features we believe to be generic. Analysis of atomic displacements associated with barrier crossing in the fragile regime suggests a scenario of correlated motions along a chain of particles as the underlying mechanism for slow viscous relaxation in glassy states.

11:51AM V39.00004 Jamming in systems with attraction1, GREGG LOIS, Yale University — Many materials jam. As density increases or temperature decreases, structural relaxation becomes sluggish and the system approaches mechanical equilibrium without spatial ordering. The concept of a universal jamming transition and the conjecture that the mechanical response at zero temperature is linked to slow dynamics at non-zero temperature has inspired research in a variety of glassy materials such as colloidal suspensions, emulsions, granular media and foams. While most recent theoretical and simulation studies of the jamming transition have focused on systems with purely repulsive interactions, many materials also possess attractive forces. I will present our recent numerical results on the jamming transition in particulate systems with attractive interactions. At zero temperature, instead of the single discontinuous jamming transition observed in purely repulsive systems, attractive systems exhibit two second-order transitions—connectivity and rigidity percolation—which belong to different universality classes than their lattice counterparts. This observation also holds for low temperature before diffusion and activation/bond-breaking become relevant. At higher temperatures, the universality class of the jamming transition can depend on the age of the system. Finally, I will discuss a proposed phase diagram for gelation and rigidification in the temperature-density plane.

1Financial support from NSF grants CTS-0348175 and DMR-0448838 is acknowledged.

12:27PM V39.00005 Is there a connection between structure and heterogeneous dynamics in supercooled liquids?2, WILLIAM KREKELBERG, VENKAT GANESAN, THOMAS TRUSKETT, University of Texas-Austin, Department of Chemical Engineering — Structurally arrested (jammed or glassy) states are prepared from supercooled fluids, though there a number of open questions regarding how that process occurs. One involves explaining why modest increases in structural order accompany the pronounced slowing of liquid-state dynamics near structural arrest. Another involves understanding why self-diffusion in deeply supercooled fluids occurs much faster than would be predicted from knowledge of the viscosity and the Stokes-Einstein relation. Single-particle displacements become heterogeneous near the glass transition, but corresponding structural heterogeneities have been difficult to identify. Collectively, these observations call into question the general prospect of understanding and predicting dynamical behavior of liquids based on structural information. In this talk, we present simulation data on several model systems that show that the dynamics of supercooled liquids can be quantitatively correlated to structure in a simple way. Specifically, we show that the breakdown of the Stokes-Einstein relationship reflects simple and distinct couplings between structure, viscosity, and diffusivity in the supercooled fluid. We also demonstrate how heterogeneous dynamics correlate with dynamically heterogeneous structure.

12:39PM V39.00006 An effective field theory for soft granular matter1, SILKE HENKES, Brandeis University, COREY O’HERN, Yale University, BULBUL CHAKRABORTY, Brandeis University — Work on packings of soft spheres (PRE 68, 011306 (2003)) has demonstrated the existence of a jamming transition and has highlighted the need for a general statistical framework to describe granular packings. We have shown that a statistical ensemble, based on conservation properties of the global stress tensor, is consistent with simulated packings of frictionless disks (PRL 99, 038002 (2007)). We construct an effective field theory based on this ensemble, in the spirit of an earlier attempt (PRL 95, 198002 (2005)). The field theory is constructed by synthesizing results from simulations into one functional form for the effective free energy. We will describe ongoing efforts to derive this form by combining scaling ideas with microscopic properties of the packings.

2Work supported by NSF-DMR 0549762.

12:51PM V39.00007 Jamming and correlated percolation on energetically-evolved graphs, SHILIANG XU, JENNIFER SCHWARZ, Physics Department, Syracuse University — Numerical simulations suggest that the zero-temperature jamming transition in repulsive soft spheres has an unusual mixed second-order/first-order character whose exponents appear to be in the same universality class as mean-field k-core percolation. In k-core percolation model, every occupied site must have at least k occupied neighbors. The k-core analogy of jamming is similar to the kinetically constrained analogy of the glass transition where the geometric constraint of k = d + 1 contacts needed for local mechanical stability drives the transition. We now introduce energetics explicitly into the analogy by investigating k-core percolation on a graph where edges are dynamically evolved with the goal of minimizing an xy-model-type interaction between a node and each of its neighbors. The xy-model-type interaction captures the angular arrangements of jammed configurations at the onset of jamming. Moreover, the graph dynamics captures nonequilibrium aspects of jamming that cannot be captured by static approaches such as a version of rigidity percolation with repulsive forces only.

1:03PM V39.00008 A “Hamiltonian” for Jammed Granular Matter, CHAOMING SONG, PING WANG, HERNAN A. MAKSE, Levich Institute and Department of Physics, City College of New York — We introduce a “Hamiltonian”-like function, called the volume function, to describe the microstates of jammed matter such as granular materials and emulsions from a geometrical point of view. We present a theory of volume fluctuations and derive the volume function defined in terms of the available free volume of the particles in the jammed systems. At the microscopic level the volume function provides an accessible “atomistic” formula for the calculation of the Voronoi volume associated with a single particle in terms of field variables. We then coarse-grain the volume function over a scale of a few particle diameters and provide a mesoscopic volume function which is now solely a function of the coordination number. We predict an exponential tail in the distribution of volumes in general agreement with experiments. Our analysis allows the calculation of macroscopic observables using the statistical mechanics of jammed states when it is supplemented by the condition of mechanical equilibrium of jamming.

1:15PM V39.00009 Vacancy localization in the square dimer model, MARK BOWICK, Syracuse University, JEREMIE BOUTTIER, EMMANUEL GUITTER, Saclay, MONWHEA JENG, Syracuse University — We study the classical dimer model on a square lattice with a single vacancy by developing a graph-theoretic classification of the set of all configurations which extends the spanning tree formulation of close-packed dimers. The motion of a vacancy induced by dimer slidings is analyzed including the size distribution of the domain accessible to the vacancy and the probability for a vacancy to be strictly jammed in an infinite system. More generally, the size distribution of the domain accessible to the vacancy is characterized by a power law decay with exponent 9/8. In a finite system, the probability that a vacancy in the bulk can reach the boundary falls off as a power law of the system size with exponent 1/2. The resultant weak localization of vacancies still allows for unbounded diffusion with a diffusion exponent related to that of diffusion on spanning trees.
1:27PM V39.00010 Velocity fluctuations in dense granular flows. JOHN DROZD, COLIN DENNISTON, University of Western Ontario — We use simulations to investigate velocity fluctuations in dry granular flow. Our system is comprised of mono- and poly-disperse sets of spherical grains falling down a vertical chute under the influence of gravity. We find three different classes of velocity distributions depending on factors such as the local density. The class of the velocity distribution depends on whether the grains are in a free-fall, fluid or glassy state. The analytic form of the distributions match those that have been found by other authors in fairly diverse systems. Here, we have all three present in a single system in steady-state. Power-law tails that match recent experiments are also found but in a transition area suggesting they may be an artifact of crossover from one class of velocity distribution to another. By studying both fast and slow flowing systems, we find that the velocity fluctuations are related to collision times by a scaling with the glass transition temperature. We measure collision time distributions along the height of the chute and find that the collision time distributions evolve from exponential tails into power-laws. This suggests that the particles may be forming clusters as they approach the glass state which may correspond to a second order dynamical phase transition.

1:39PM V39.00011 Energy Transport of Jammed Systems1. NING XU, University of Pennsylvania and University of Chicago, VINCENTI VITELLI, University of Pennsylvania, MATTHIEU WYART, Harvard University, ANDREA LIU, University of Pennsylvania, SIDNEY NAGEL, University of Chicago — We perform computer simulations to calculate the thermal conductivity of vibrational modes in jammed sphere packings near the jamming transition (Point J). The diffusivity d(ω) is low for all modes, including those at low frequency ω, and appears to be finite in the zero frequency limit. In ordinary solids, by contrast, d(ω) diverges at low frequencies due to long wavelength plane waves. The low- frequency modes near Point J are very different from plane waves: they are quasi-localized with large anharmonic corrections. Thus, these modes, which can be viewed as harmonic precursors to two-level systems, are poor conductors of energy.

1:51PM V39.00012 Testing ergodicity in dense granular systems. GUO-JIE GAO, JERZY BLAWZDZIEWICZ, COREY O’HERN, Yale University — The Edwards’ entropy formalism provides a statistical mechanical framework for describing dense granular systems. Experiments on vibrated granular columns and numerical simulations of quasi- static shear flow of dense granular systems have provided indirect evidence that the Edwards’ theory may accurately describe certain aspects of these systems. However, a fundamental assumption of the Edwards’ description—that all mechanically stable (MS) granular packings at a given packing fraction and externally imposed stress are equally accessible—has not been explicitly tested. We investigate this assumption by generating all mechanically stable hard disk packings in small bidisperse systems using a protocol where we successively compress or decompress the system and then record the MS packings that occur during the shear flow. We generate a complete library of the allowed MS packings at each value of shear strain and determine the frequency with which each MS packing occurs. We find that the MS packings do not occur with equal probability at any value of shear strain. In fact, in small systems we find that the evolution becomes periodic with a period that grows with system-size. Our studies show that ergodicity can be improved by either adding random fluctuations to the system or increasing the system size.

2:03PM V39.00013 Anomalously Slow Dynamics in the Manhattan Model1. PRASANTA PAL, Department of Applied Physics, Yale University, COREY O’HERN, Department of Mechanical Engineering, Yale University — We study the Brownian dynamics of hard rods in a Manhattan-like traffic grid, in which a series of narrow horizontal and vertical channels intersect at right angles and particles are forbidden from turning at the intersections. We measure the mean-square displacement (msd) as a function of packing fraction φ and determine the δφ at which dynamical arrest occurs as a function of system size, number of intersections, and topology of the grid. We observe that structural relaxation occurs via a complex out-of-equilibrium process in which particles occupy locally dense regions of the grid and then undergo a first passage process. We compare our results for the msd and δφ to that found in model glass-forming liquids in two and three dimensions.

1Supported by DE-FG02-05ER46199 and DE-FG02-03ER46088

2Supported by grant number NSF-CBET0625149 is acknowledged.

Thursday, March 13, 2008 11:15AM - 2:15PM
Session V40 DBP: Nucleic Acids: Structure and Function Morial Convention Center 232

11:15AM V40.00001 Toward multiscale modeling of the chromatin fiber: a coarse grain model for DNA. ALEXEY SAVELYEV, GAREGIN PAPOIAN, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599-3290 — In eukaryotic cells DNA is compacted a million-fold into a chromatin. Understanding the mechanism of chromatin folding is of great biological importance. All-atom Molecular Dynamics (MD) simulations could provide crucial insights into the electrostatic and structural mechanisms of chromatin folding. However, because of the enormous size of even short chromatin fiber segment and long folding time-scales, atomistic simulations are computationally impractical. Our long-term aim is to build an accurate coarse-grain (CG) model of the chromatin, derived systematically from all-atom simulations of its smaller parts. Here we report the development of the CG model for a linear DNA chain, playing the role of a linker DNA segment in the chromatin. We derived CG inter-DNA electrostatic potential from atomistic simulations with explicit solvent and mobile ions, instead of relying on the standard models of continuum electrostatics, which are inadequate at small intermolecular distances. In addition, we used the ideas of renormalization group theory to construct an optimization scheme to parameterize the CG force field. This novel approach is designed to accurately reproduce correlations among various CG degrees of freedom. The implementation of these correlations was left as an open question in the prior studies of CG polymer models.

11:27AM V40.00002 Sequence and Temperature Dependence of DNA Bending Fluctuations. ROBERT A. FORTIES, RALF BUNDSCHUH, MICHAEL G. POIRIER, Department of Physics, The Ohio State University, 191 West Woodruff Avenue, Columbus, Ohio 43210-1117, USA — Recent DNA cyclization experiments measured J factors indicating that DNA may form sharp bends more easily than predicted by the worm-like chain model. One proposed explanation is that local melting of a few base pairs (bp) introduces flexible hinges [Yan, J. et al., Phys. Rev. E 71, 061905 (2005)]. We incorporate sequence dependence of the local melting into this model and obtain specific predictions for the dependence of J factors on temperature and sequence. We then measure J factors for a 200 bp fragment of lambda DNA and two synthetic 116 bp sequences with different proclivities for melting. The measured temperature and sequence dependence of J factors is found to be in agreement with the sequence dependent model predictions using previously measured free energy costs for melting and reasonable estimates for the flexibility of melted segments of DNA.

11:39AM V40.00003 Mechanically unzipping dsDNA with built-in sequence inhomogeneities and bound proteins. ABHIJIT SARKAR, Virginia State University — We theoretically analyze the force signal from unzipping dsDNA with bound proteins and sequence inhomogeneities. Two different force traces are obtained determined by binding and sequence parameters. Sawtooth force curves, as observed in experiments, are found for short enough designed sequences and binding sites. Longer inhomogeneities lead to force plateaus which correspond to gradual, piece-meal, unzipping of the variant stretch of DNA. We generalize our model to allow comparisons to recent experiments on unzipping decorated DNAs.
The elastic properties of the DNA molecule are important for its function. On a base-pair scale, they modulate protein binding strength, while over hundreds of base-pairs, they govern the statistics of DNA loops. We have used the rigid base–pair (RBP) model to link experiments on DNA elasticity across these scales. In a study of the indirect readout mechanism in protein–DNA binding, we compare calculated DNA elastic free energy differences to experimental affinities. While quantitative predictions are beyond the precision of current parameter sets, qualitative predictions are meaningful; we propose a statistical marker for indirect readout sub-sites in a given co-crystal geometries produced by the CH$_3$ group. More quantitative results from our current investigations using the actual sugar rings and phosphate groups will be presented as in earlier work by our group[1] for hyperfine interactions of trapped muonium atoms in DNA.

In recent work [1] we have studied nucleobases attached to a CH$_3$ group to simulate the influence of their binding to the sugar rings and the phosphate groups in DNA and RNA and the effect of this binding on the nuclear quadrupole interactions of $^{14}$N, $^{17}$O and $^2$H nuclei. Our results from this work have indicated that for $^{17}$O, the binding to the CH$_3$ group moves our results from the free nucleobases closer to the experimentally observed data [2] in the solid nucleobases. We are now investigating the solid nucleobases by the first–principles Hartree-Fock cluster procedure that we have employed earlier for the halogen molecular solids [3]. Our results for the binding energy of an imidazole molecule in the molecular solid system and the $^{14}$N, $^{17}$O and $^2$H quadrupole interaction parameters will be presented.

We have first simulated the influence of the interaction between a nucleobase and a sugar ring using a CH$_3$ group attached to the former. For our electronic structure investigations, we have employed the Hartree-Fock–Roothaan procedure using the Gaussian set of programs. Our preliminary investigations have shown that there are comparable indirect and direct effects on the NQI parameters, the former effect referring to the influence of changes in molecular geometries produced by the CH$_3$ group and the direct effect is due to the electronic interaction between the CH$_3$ group and the nucleobase. More quantitative results from our current investigations using the actual sugar rings and phosphate groups will be presented as in earlier work by our group[1] for hyperfine interactions of trapped muonium atoms in DNA.[1] R.H. Scheicher et al Physica B 374-375 (2006).

1 Work supported by Monbusho
2 Tsudanuma, Narashino-shi, Chiba 275

2:03PM V40.00015 Simplified Hamiltonians for coarse-grained properties of large single-stranded RNA molecules, PETER PRINSEN, ARON YOFFE, WILLIAM GELBART, Department of Chemistry and Biochemistry, UCLA — Large single-stranded RNA (ssRNA) molecules with a length of a few thousand to a few tens of thousands of nucleotides are quite common in nature. These RNAs generally have a highly branched secondary structure with many short, double-stranded sections. The secondary structure is important for function. However, the prediction of the thermally accessible secondary structures of large ssRNAs is complicated. There are several computer programs available that predict secondary structures of ssRNA. They produce good results for small molecules but are not very reliable for large ones. We are not interested in "high-resolution" structures, however, but in more coarse-grained properties, for example the average three-dimensional size of the molecule. We expect that the available computer programs are useful for determination of these coarse-grained properties but the complicated Hamiltonians they use limit the usefulness of these models for further theoretical investigations. We show that one can simplify these Hamiltonians considerably and still retain important predictive power. The inclusion of stacking energies is crucial but many of the detailed energy rules are not. We define several measures for the size of a secondary structure and we show how these measures are related to each other.

Thursday, March 13, 2008 2:30PM - 4:54PM —
Session W2 DCMP: Electronic Structure, Magnetism and Superconductivity of Sodium Cobaltate
Morial Convention Center LaLouisiane C
We show that the potential. We find a class of charge and spin density ordered states where the system alleviates antiferromagnetic (AF) frustration via charge inhomogeneity [2].

Coulomb repulsion renormalizes the crystal field splitting and the bandwidths of the t, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA 02467 — We argue that the strong Co intra-atomic evidence for charge ordering in the insulating ground state of Na
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Role of strong correlation and Na dopant order, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA 02467 — We argue that the strong Co intra-atomic Coulomb repulsion normalizes the crystal field splitting and the bandwidths of the t2g complex in Na2CoO2, resulting in a single band crossing the Fermi level at all doping levels x explored by ARPES experiments [1]. On this basis, we study the electronic states using a minimal electron-doped, one-band Hubbard model with large U on the triangular lattice. The important role played by the off-plane Na dopants is taken into account by including the ionic electrostatic potential. We find a class of charge and spin density ordered states where the system alleviates antiferromagnetic (AF) frustration via charge inhomogeneity [2]. We show that the √3×2 Na order at x = 0.5 causes weak √3×1 charge order in the Co layer and the emergence of AF order with small electron and hole Fermi surface pockets [2]. This theory of the “0.5 phase” is consistent with neutron scattering, NMR, Shubnikov-de Haas oscillations, and transport experiments. In the sodium rich phases, the high density of off-plane Na dopants (or dilute Na vacancies), in their ordered or disordered form, increases the tendency toward strongly correlated electron behavior as a function of sodium concentration x, ranging from itinerant antiferromagnet (x∼0.84 and 0.5), “Curie-Weiss metal” (x∼0.71) to Fermi liquid (x∼1/3). In this talk, I will discuss our NMR studies of Na2CoO2 for various Na concentration x, with particular emphasis on 59Co evidence for charge ordering in the insulating ground state of NaN5Co2O2 [1-4].

4:18PM W2.00004 Novel electronic states in Na2CoO2: Role of strong correlation and Na dopant order, ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA 02467 — We argue that the strong Co intra-atomic Coulomb repulsion normalizes the crystal field splitting and the bandwidths of the t2g complex in Na2CoO2, resulting in a single band crossing the Fermi level at all doping levels x explored by ARPES experiments [1]. On this basis, we study the electronic states using a minimal electron-doped, one-band Hubbard model with large U on the triangular lattice. The important role played by the off-plane Na dopants is taken into account by including the ionic electrostatic potential. We find a class of charge and spin density ordered states where the system alleviates antiferromagnetic (AF) frustration via charge inhomogeneity [2]. We show that the √3×2 Na order at x = 0.5 causes weak √3×1 charge order in the Co layer and the emergence of AF order with small electron and hole Fermi surface pockets [2]. This theory of the “0.5 phase” is consistent with neutron scattering, NMR, Shubnikov-de Haas oscillations, and transport experiments. In the sodium rich phases, the high density of off-plane Na dopants (or dilute Na vacancies), in their ordered or disordered form, increases the tendency toward strongly correlated electron behavior as a function of sodium concentration x, ranging from itinerant antiferromagnet (x∼0.84 and 0.5), “Curie-Weiss metal” (x∼0.71) to Fermi liquid (x∼1/3). In this talk, I will discuss our NMR studies of Na2CoO2 for various Na concentration x, with particular emphasis on 59Co evidence for charge ordering in the insulating ground state of NaN5Co2O2 [1-4].

References:
[1]. F.L. Ning et al., arXiv: 0711.4023
[4]. F.L. Ning et al., arXiv: 0709.0085

Thursday, March 13, 2008 2:30PM - 4:54PM —
Session W3 DCMP: Dislocation Patterns and Avalanches Morial Convention Center RO2 - RO3

2:30PM W3.00001 Scale-Free Intermittent Flow in Crystal Plasticity, RICHARD LESAR, Iowa State University — Under stress, crystals irreversibly deform through complex dislocation processes — processes that intermittently change the microscopic material shape through isolated slip events. Using both model computer simulations and ultra-precise nano-scale measurements on nickel micro-crystals we directly determined the size of discrete slip events. The sizes range over nearly three orders of magnitude, and exhibit a shock and aftershock earthquake-like behavior over time. Analysis of the events reveals power-law scaling between the number of events and their magnitude, or scale-free flow. We show that dislocated crystals are a model system for studying scale-free behavior that is observed for many macroscopic systems. By analogy to plate tectonics, smooth macroscopic-scale crystalline glide arises from the spatial and time averages of disruptive earthquake-like events at the nano-scale.
Dislocations with glide only support minimal domain formation. The talk will enumerate various PTV studies of step shear, startup shear and large-amplitude oscillatory shear to show how these crucial experiments have produced step deformation. The transient cohesion provided by chain entanglement due to inter-molecular interactions is found to be higher at a higher applied rate. This take place inhomogeneously in both shear and extension. Most remarkably, an entangled polymer would suffer “delayed” cohesive structural breakdown after a velocimetric observations (PTV, which are available for downloading at http://www3.uakron.edu/rheology/) show that the elastic yielding and subsequent flow than the relaxation rate of entangled chains, a well entangled polymeric liquid yields like a solid before being forced to flow plastically. Recent particle tracking rate that is a sensitive function of molecular weight and its distribution. At high Weissenberg number, i.e., when the rate of external deformation is far greater than the stress relaxation time of entangled chains, a well entangled polymeric liquid relaxes like a solid before being forced to flow plastically.

CR motion was found to be valid for blends and star chains. Even for this case, the tube diameter increases to a level accepted by the CR motion. The partial-DTD picture considering this consistency with the increase of the fully dilated tube diameter over which the CR motion of the probe cannot occur in time, which naturally results in the failure of the full-DTD comparison indicated that the full-DTD picture works satisfactorily for monodisperse linear PI but not for blends of linear PI as well as for monodisperse star PI.

This constant ratio simply results from an implicit coarse-graining procedure that is performed upon measuring different types of quantities in the simulated picture. Even for this case, the tube diameter increases to a level accepted by the CR motion. The partial-DTD picture considering this consistency with the increase of the fully dilated tube diameter over which the CR motion of the probe cannot occur in time, which naturally results in the failure of the full-DTD comparison indicated that the full-DTD picture works satisfactorily for monodisperse linear PI but not for blends of linear PI as well as for monodisperse star PI.

The effective diffusion constant decayed to zero as: $D(t)=D(0)e^{-t/\tau}$, with $\tau=0.8$. Coarsening: Dislocations with glide and climb exhibited profound domain formation, the domains coarsen as $L(t): L(t) \sim t^{1/2}$, with $1/2=0.17$. The formation of domains without shear has been recently observed in GaAs by Rudolph and in dusty plasmas by Quinn and Joree. The domain coarsening was quantitatively captured in di-block copolymers [2], with $1/2=0.19$, in good agreement with our results.


3:42PM W3.00003 Domain Coarsening and Aging in Dislocation Glasses 1, GERGELY ZIMANYI, Physics Department, UC Davis — Dislocation systems were analyzed numerically with 1 and 3 glide axes, at T=0 and T>0, with and without climb. [1] Dislocation free domains formed even without shear, defined by dislocation rich domain walls. The domain formation was most pronounced in the presence of climb, somewhat counter-intuitively. The stability of domains was analyzed. The microscopic processes suppressing the climb-induced decay of domain walls were identified. The dislocation dynamics at low temperatures was markedly glassy. Aging: Dislocations with glide only support minimal domain formation. The autocorrelation function showed aging, scaling with the waiting time as: $C(t,t_0)=C_0(t/t_0^\gamma)$ and $C_0(t) \sim t^{-\beta}$, with $\mu=0.65$ and $\beta=0.54$. Freezing: The effective diffusion constant decayed to zero as: $D(t)e^{\gamma} \sim t^{-\gamma}$, with $\gamma=0.8$. Coarsening: Dislocations with glide and climb exhibited profound domain formation, the domains coarsen as $L(t)$: $L(t) \sim t^{1/2}$, with $1/2=0.17$. The formation of domains without shear has been recently observed in GaAs by Rudolph and in dusty plasmas by Quinn and Joree. The domain coarsening was quantitatively captured in di-block copolymers [2], with $1/2=0.19$, in good agreement with our results.


4:18PM W3.00004 Dislocation Avalanches, Mean Free Path and Patterning 1, L.P. KUBIN, LEM, CNRS-ONERA, 29 Av. de la Division Leclerc, BP72, 92322 Châtillon Cedex, France — Dislocations are the defects that carry plastic flow in crystalline materials. At the defect scale, plastic deformation occurs by dislocation avalanches, which are characterized by scale-free behavior within a bounded domain of amplitudes or energies. The probability distribution functions of these avalanches, their processes of initiation and termination and their contribution to dislocation storage during plastic flow are investigated dislocation dynamics (DD) simulations. The model material is a copper single crystal strained along three high symmetry orientations. The distributions of avalanche amplitudes exhibit, for all orientations, a scaling exponent of 1.6, similar to what is reported in the literature. However, the average value of strain burst amplitudes, taken in the recorded domain of amplitudes, is found to be orientation-dependent. In parallel, a continuum model based on the notion of dislocation mean free path, which predicts the mechanical response of f.c.c. single crystals, was established with the help of DD simulations. It appears that both intermittent and continuum behavior exhibit the same orientation dependencies. Furthermore, for the three tested orientations, the ratio of the continuum mean free path to the average characteristic length traveled by dislocations during avalanches is a constant. This constant ratio simply results from an implicit coarse-graining procedure that is performed upon measuring different types of quantities in the simulated results. As a consequence, it appears that avalanche behavior can effectively be incorporated into continuum models for plasticity. The present results are discussed with respect to the available experimental literature on the deformation of f.c.c. crystals. Finally, the formation of dislocation patterns, that is the self-organization properties of dislocations under strain, is tentatively discussed in terms of the properties of dislocation avalanches.


Thursday, March 13, 2008 2:30PM - 5:30PM — Session W4 DPOLY: Dynamics of Polymers Morial Convention Center 206

2:30PM W4.00001 Dielectric and Viscoelastic Investigation of Entanglement Relaxation, HIROSHI WATANABE, Kyoto University — For a chain (probe) entangled with surrounding chains (matrix), the entanglement is released on large-scale motion of the matrix chains. This constraint release (CR) mechanism plays a central role in the current tube model for entangled chains. Since the distance for the lateral motion of the probe (= tube diameter) increases on CR, the tube model often utilizes the molecular picture of dynamic tube dilation (DTD) to represent the CR effect on the probe dynamics. In the simplest case of full-DTD, the relaxed portion behaves as a solvent giving no constraint and the tube diameter increases to the diameter in the corresponding solution. This talk utilizes cis-polysisoprene (PI) having the type-A dipole to test the validity of the DTD picture with the following strategy. The type-A dipole allows us to dielectrically evaluate the survival fraction f(t) of the diluted tube at time t. The full-DTD picture can be unequivocally tested by comparing the normalized viscoelastic modulus deduced from this picture (2.0-2.3h power of f(t)) with the viscoelastic data. The comparison indicated that the full-DTD picture works satisfactorily for monodisperse linear PI but not for blends of linear PI as well as for monodisperse star PI. The failure of the full-DTD picture for the last two systems is related to the fast relaxation modes in these systems. These modes lead to a significant increase of the fully diluted tube diameter over which the CR motion of the probe cannot occur in time, which naturally results in the failure of the full-DTD picture. Even for this case, the tube diameter increases to a level accepted by the CR motion. The partial-DTD picture considering this consistency with the CR motion was found to be valid for blends and star chains.

3:06PM W4.00002 How does cohesive breakdown occur in entangled polymeric liquids? 1, SHIQING WANG, Department of Polymer Science, University of Akron — Entangled polymers are strongly viscoelastic materials with a characteristic relaxation rate that is a sensitive function of molecular weight and its distribution. At high Weissenberg number, i.e., when the rate of external deformation is far greater than the relaxation rate of entangled chains, a well entangled polymeric liquid yields like a solid before being forced to flow plasticly. Recent particle tracking velocimetric observations (PTV, which are available for downloading at http://www3.uakron.edu/rheology/) show that the elastic yielding and subsequent flow take place inhomogeneously in both shear and extension. Most remarkably, an entangled polymer would suffer “delayed” cohesive structural breakdown after a step deformation. The transient cohesion provided by chain entanglement due to inter-molecular interactions is found to be higher at a higher applied rate. This talk will enumerate various PTV studies of step shear, startup shear and large-amplitude oscillatory shear to show how these crucial experiments have produced a phenomenological level understanding (J. Chem. Phys. 2007, 127, 064903) of various flow phenomena in entangled polymers.

1 In collaboration with: Pouyam Boukany, Sham Ravindranath, Yangyang Wang, Department of Polymer Science, University of Akron.
4:18PM W4.00004 Shear Alignment and Realignment of Block Copolymer Microdomains in Thin Films1, RICHARD REGISTER, Princeton University — Bulk block copolymers, like all liquid crystalline structures, are well-known to align under flow. In the past few years, we have shown that analogous flow alignment can be achieved in substrate-supported thin films (<100 nm thick) containing one or a few layers of spherical or cylindrical nanodomains. Alignment can easily be imparted either by pulling a soft rubber pad in contact with the top surface of the film, or by flowing a nonsolvent fluid across the film. The latter geometry opens the possibility to “write” relatively complex patterns on the millimeter or submillimeter scale, where the nanodomain director follows the fluid streamline. Alignment can be achieved via either unidirectional or oscillatory shear, and is conveniently executed in a parallel-plate rheometer, where the substrate-supported film forms one “plate” and the “gap” is filled with the nonsolvent fluid. A threshold stress is required to achieve alignment of the microdomains, a stress which decreases steadily as the temperature is raised towards the polymer’s order-disorder transition temperature. A simple melting-recrystallization model appears to capture the dynamics of overall alignment. Though no grain boundaries remain in well-aligned films, isolated dislocations persist. For sphere-formers, where two or more layers are required for alignment, the isolated dislocations are preferentially oriented in such a way as to facilitate sliding of the two layers of spheres past each other. Once a macroscopic orientation has been imparted to the film (over square-cm area), the microdomains can be reoriented by applying shear in a different direction, but a higher threshold stress is required than was needed for the initial alignment from the polycrystal state. Recently, we have observed a sphere-to-cylinder transition in one particular block copolymer under shear, opening another possible mechanism for shear-induced alignment of the spheres which form when these cylinders relax.

1 with Andrew Marencic, Young-Rae Hong, Mingshaw Wu, Vincent Pelletier, Douglas Adamson, and Paul Chaikin, supported by the NSF MRSEC Program through the Princeton Center for Complex Materials (DMR-0213706)

4:54PM W4.00005 Nanoparticle Ionic Liquids, LYNDEN ARCHER, School of Chemical and Biomolecular Engineering — Nanoparticle ionic liquids (NIMS) are a new class of organic-inorganic hybrid materials comprised of a nanoparticle core functionalized with a covalently-attached organic corona. These materials manifest a remarkable transition to a “solvent-free” colloidal liquid state near room temperature. Physical properties of these nanoparticle ionic liquids can be manipulated over an unusually wide range by varying geometric and chemical characteristics of the inorganic core and organic corona. On one end of the spectrum are materials with a high core particle contents, which display properties similar to fragile glasses, stiff waxes, and gels. At the opposite extreme are systems that spontaneously form particle-based ionic fluids characterized by transport properties remarkably similar to simple molecular liquids, but with high dielectric constants, conductivities, and refractive index. This talk will introduce nanoparticle ionic fluids based on charged and uncharged corona species, explore their applications, and will discuss physical and mathematical models for understanding their interactions, complex relaxation dynamics, and rheology.

Thursday, March 13, 2008 2:30PM - 5:30PM – Session W5 FIAP: Sensing Science and Sensors for Industrial Applications Morial Convention Center R01

2:30PM W5.00001 Next-Generation Mid-Infrared Chemical Sensors Challenges and Opportunities, BORIS MIZAIKOFF, Georgia Institute of Technology — No abstract available.

3:06PM W5.00002 Laser Interferometry for Harsh Environment MEMS Sensors, PATRICIA NIEVA, University of Waterloo — Silicon-based MEMS technology has enabled the fabrication of a broad range of sensor and actuator systems that are having a great impact in areas that benefit from miniaturization and increased functionality. The main advantage of Si-based MEMS technologies is their possibility of integration with microelectronics thus allowing the economical production of smart Microsystems. In the automotive industry for example, there is a need for inexpensive smart MEMS sensors for engine control applications. For instance, smart MEMS sensors capable of operating “in cylinder”, where temperatures are around 400 °C, could continuously monitor the combustion quality of the cylinders of automotive engines thus leading to reduced emissions and improved fuel economy. However, when the environment temperature is too high (>180 °C), conventional Si-based microelectronics suffer from severe performance degradation, thus making smart Si-based MEMS impractical. Hence, further development, in terms of new MEMS materials and/or new technologies, is needed especially where high temperature capability is crucial to realizing improved electronic control. Remote sensing through optical signal detection has major advantages for safe signal transmission in harsh environments. It is highly resistant to electromagnetic interference (EMI) and radio frequency interference (RFI) and at the same time, it eliminates the necessity of on-board electronics, which has been one of the main obstacles in the development of smart MEMS sensors for high temperature applications. An economical way to deal with higher temperatures and other aggressive environmental conditions is to build MEMS sensors out of robust materials (e.g. Silicon nitride, SiC) and integrate them with optical signal detection techniques to form MOEMS. In this paper, we review recent trends for the use of laser interferometry for MEMS sensors in the context of using them for high temperature applications. Technological challenges faced in the development of these sensors, including sensitivity to measurement errors, packaging and cost reduction are also outlined. Finally, an overview of Fabry-Perot like MEMS sensors for high temperature applications is presented and issues facing their future progress and economical implementation are discussed.

3:42PM W5.00003 Chemical and Physical Sensing in the Petroleum Industry, MARK DISKO, ExxonMobil Research & Engineering Company — World-scale oil, gas and petrochemical production relies on a myriad of advanced technologies for discovering, producing, transporting, processing and distributing hydrocarbons. Sensing systems provide rapid and targeted information that can be used for expanding resources, improving product quality, and assuring environmentally sound operations. For example, equipment such as reactors and pipelines can be operated with high efficiency and safety with improved chemical and physical sensors for corrosion and hydrocarbon detection. At the interface between chemical engineering and multiphase flow physics, “multi-scale” phenomena such as catalysis and heat flow benefit from new approaches to sensing and data modeling. We are combining chemically selective micro-cantilevers, fiber optic sensing, and acoustic monitoring with statistical data fusion approaches to maximize control information. Miniaturized analyzers represent a special opportunity, including the nanotech-based quantum cascade laser systems for mid-infrared spectroscopy. Specific examples for use of these new micro-systems include rapid monomeric aromatic molecule identification and measurement under ambient conditions at weight ppb levels. We also propose from emerging materials and devices based on nanotechnology, which can one day be available at modest cost for impact in existing operations. Controlled surface energies and emerging chemical probes hold the promise for reduction in greenhouse gas emissions for current fuels and future transportation and energy technologies.
4:18PM W5.00004 Silicon Carbide Micro/Nano Systems for Demanding and Harsh Environment Applications, MEHRAN MEHREGANY, Department of Electrical Engineering and Computer Science, Case Western Reserve University, Cleveland, Ohio 44106 — Micro/nano systems enable the development of smart products and systems by augmenting the computational ability of microelectronics with the perception and control capabilities of sensors and actuators. Micro/nano systems are also known as micro- and nanoelectromechanical systems (MEMS and NEMS), and have been commercialized in a wide range of applications including crash sensing, blood pressure measurement, optical projection, and fluid flow control to name a few. Silicon, in single- and polycrystalline forms, has been the platform semiconductor material underpinning the fabrication of the mechanical and electronic elements of micro/nano systems. However, the materials properties of silicon impose limitations on its use in harsh environment and demanding applications—for example, those involving operation in the presence of high temperatures, corrosive media, high shock loads, erosive flows, and/or high radiation, or involving performance requirements for the mechanical elements that are beyond silicon’s capabilities. Silicon carbide (SiC) is an alternative platform semiconductor material that enables such applications because of its wider bandgap and higher melting/sublimation temperature, elastic modulus, fracture toughness, hardness, chemical inertness, and thermal conductivity. This talk will highlight our most recent SiC material, process, and device advances to enable sensing and actuation in applications such as propulsion instrumentation/control, power generation, resource exploration, nuclear reactor instrumentation, deep space exploration, and communications.

4:54PM W5.00005 SiC Sensors in Extreme Environments: Real-time Hydrogen Monitoring for Energy Plant Applications1, RUBY GHOSH2, Michigan State University — Clean, efficient energy production, such as the gasification of coal (syngas), requires physical and chemical sensors for exhaust gas monitoring as well as real-time control of the combustion process. Wide-bandgap semiconducting materials systems can meet the sensing demands in these extreme environments consisting of chemically corrosive gases at high temperature and pressure. We have developed a SiC-based micro-sensor for detection of hydrogen containing species with millisecond response at 600 °C. The sensor is a Pt-SiO2-SiC device with a dense Pt catalytic sensing film, capable of withstanding months of continuous high temperature operation. The device was characterized in robust sensing module that is compatible with an industrial reactor. We report on the performance of the SiC sensor in a simulated syngas ambient at 370 °C containing the common interferants CO2, CH4 and CO [1], and in addition demonstrate that hours of exposure to ≥1000 ppm H2S and 15% water vapor does not degrade the sensor performance. To elucidate the mechanisms responsible for the hydrogen response of the sensor we have modeled the hydrogen adsorption kinetics at the internal Pt-SiO2 interface, using both the Tempkin and Langmuir isotherms. Under the conditions appropriate for energy plant applications, the response of our sensor is significantly larger than that obtained from ultra-high vacuum electrochemical sensor measurements at high temperatures. We will discuss the role of morphology, at the nano to micro scale, on the enhanced catalytic activity observed for our Pt sensing films in response to a heated hydrogen gas stream at atmospheric pressure.


1This work was supported by the National Energy Technology Lab of DOE.
2Collaborators: R. Loloee & B. Chorpening.

Thursday, March 13, 2008 2:30PM - 5:30PM –
Session W6 DAMOP: Strong Interacting Fermi Gases with Spin Asymmetry
Morial Convention Center

2:30PM W6.00001 Experiments in spin-polarized Fermi gases—pairing without superfluidity?
CHRISTIAN SCHUNCK, Massachusetts Institute of Technology — Fermionic superfluidity requires pairing of fermions. The nature of fermionic pairing in the strongly interacting regime both in the superfluid and possibly in the normal phase is of interest to condensed matter, nuclear and high energy physics. The experimental realization of high temperature superfluidity in ultracold Fermi gases opens a new approach to explore strongly interacting fermions both in the superfluid and normal phases. One question of relevance for example to superfluidity of quark’s in cold baryonic matter as well as superconductivity has been the stability of the superfluid against an imbalance between the two strongly interacting fermionic components. An imbalance can be caused by different masses of the fermions or an externally applied magnetic field to a superconductor. In our experiments a density imbalance between two fermionic spin components is introduced. We will present the phase diagram of a spin-polarized Fermi gas of 6Li atoms at unitarity, mapping out the superfluid phase versus temperature and density imbalance. The nature of the phase transition changes from first-order to second-order at a tricritical point. At zero temperature, there is a quantum phase transition from a fully-paired superfluid to a partially-polarized normal gas at a critical spin polarization, known the Chandrasekhar-Clogston limit of superfluidity. These observations together with the implementation of an in situ ideal gas thermometer provide quantitative tests of theoretical calculations on the stability of resonant superfluidity. Pairing correlations in the superfluid and normal phases were explored in radio-frequency spectroscopy experiments. We studied how pairing correlations evolve across the superfluid to normal phase transition both as a function of temperature and spin imbalance. Even at spin imbalances above the Chandrasekhar-Clogston limit a gap in the single-particle excitation spectrum is observed. This indicates that the system is in a correlated state and the minority component is paired. The influence of final state interactions on the rf spectra will be discussed. Using a new superfluid 6Li spin mixture we demonstrate that pair dissociation spectra in the BEC-BCS crossover resemble asymmetric molecular dissociation spectra. Work done in collaboration with Y. Shin, A. Schiroztek and W. Ketterle, Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, MIT, Cambridge, MA 02139.

3This work was supported by the NSF, ONR and through a MURI and DARPA program.

3:06PM W6.00002 Theory of RF Spectroscopy in Strongly Interacting Fermi Gases1, ERICH MUELLE, Cornell University — Radio frequency (RF) spectroscopy is an extremely powerful probe of the many-body state of a gas of cold atoms. For example spectra of cold Fermi gases have been used as evidence of superfluidity, and of pairing fluctuations in the normal state. Despite the large amount of information they contain, spectra of trapped gases are not completely trivial to analyze. I will discuss the theory of RF spectroscopy, showing that the link between pairing and the observed spectra is very indirect, and that many of the “pairing” features occur even in a gas with no pairing whatsoever. I will also describe the important role played by final state interactions.

1Work supported in part by NSF Grant PHY-0456261.
3:42PM W6.00003 Phase separation in a spin polarized Fermi gas at the BEC-BCS crossover1, GUTHRIE PARTRIDGE, Rice University — A strongly interacting ultra-cold gas of fermionic \textsuperscript{\textit{6}}Li with unequal numbers of two spin components exhibits two distinct low temperature paired states.\textsuperscript{2} Phase separation, where a uniformly paired core is maintained in the center of the trap by the expulsion of excess unpaired atoms, is observed at the lowest temperatures up to large number imbalance. Sharp boundaries, consistent with a first-order phase transition, are observed between the core and the unpaired atoms. Moreover, the superfluid core deforms markedly, becoming less elongated due to surface tension at the superfluid/normal boundary. At higher temperature, the core remains unpolarized up to a critical polarization, but does not deform. This temperature dependence is consistent with a tri-critical point in the phase diagram. Additionally, we are exploring the possibility that the large critical imbalance for loss of phase separation is a result of relatively small particle number (10\textsuperscript{10}) and high aspect ratio (30) elongated confinement.

To date, no evidence for the long sought Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state has been observed in ultracold atomic gases. It is predicted that in 3D the FFLO phase occupies a very small region of the phase diagram,\textsuperscript{3} whereas in 1D, the stability of the FFLO state is believed to be enhanced. Though the current optical potential is elongated, it is still in the 3D regime, and so a 2D optical lattice potential has been constructed to provide an array of 1D tubes. We will present results of our studies of the polarized Fermi gas in this 1D geometry.

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4:18PM W6.00004 Few-body physics of trapped unequal mass fermions\textsuperscript{1}, CHRIS H. GREENE, Department of Physics and JILA, University of Colorado, Boulder, CO 80309-0440 — The behavior of a two-component dilute Fermi gas exhibits an interesting dependence on the mass ratio between the two species. Our study tackles this system with 3-20 particles, using two independent techniques. First, an essentially exact diagonalization for 3-6 particles determines both the ground state and also the pattern of excited state energies, and our analysis permits an extraction of the dimer-dimer scattering length and effective range. Secondly, the nature of the system ground state is studied as a function of the mass ratio and the number of particles, up to N=20, using fixed-node diffusion Monte Carlo (DMC) techniques. By using different solution techniques in their overlapping range of applicability from N=3-6, we are able to assess the accuracy of the nodal surface employed in the fixed-node DMC calculation. Physical properties such as the excitation gap will be analyzed over this range of particle number, and the intriguing unitarity limit is also considered.

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4:54PM W6.00005 Exploring an ultracold Fermi-Fermi mixture: interspecies Feshbach resonances of \textsuperscript{\textit{6}}Li-\textsuperscript{\textit{40}}K, FLORIAN SCHRECK, Oesterreichische Akademie der Wissenschaften — We report on the observation of interspecies Feshbach resonances in an ultracold mixture of two fermionic species, \textsuperscript{\textit{6}}Li and \textsuperscript{\textit{40}}K. Interpretation of the data unambiguously assigns molecular bound states to the various resonances and fully characterizes the ground-state scattering properties in any combination of spin states. Using this knowledge we hope to be able to produce \textsuperscript{\textit{6}}Li-\textsuperscript{\textit{40}}K molecules, cool them to quantum degeneracy, and study their BEC-BCS crossover.

In collaboration with: F. Schreck, Institut fuer Quantenoptik und Quanteninformation, Oesterreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria; E. Wille, Institut fuer Quantenoptik und Quanteninformation, Oesterreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria and Institut fuer Experimentalphysik und Forschungszentrum fuer Quantenphysik, Univeristat Innsbruck, 6020 Innsbruck, Austria; F.M. Spiegelhalder, G. Kerner, D. Naik, A. Trenkwalder, G. Hendi, Institut fuer Quantenoptik und Quanteninformation, Oesterreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria; R. Grimm, Institut fuer Quantenoptik und Quanteninformation, Oesterreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria and Institut fuer Experimentalphysik und Forschungszentrum fuer Quantenphysik, Univeristat Innsbruck, 6020 Innsbruck, Austria; T.G. Tiecke, J.T.M. Walraven, Van der Waals-Zeeman Institute of the University of Amsterdam, 1018 XE, The Netherlands; S.J.J.M.F. Kokkelmans, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands; E. Tiesinga, P.S. Julienne, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, Maryland 20899-8423, USA.

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2:30PM W7.00001 Representing Information with Correlated Neural Populations\textsuperscript{1}, MICHAEL BERRY, Princeton University — Using a multi-electrode array, we can record simultaneously from up to 50 ganglion cells, the output neurons of the retina, while stimulating with varied visual images generated on a computer monitor. We find that nearby ganglion cells, the output neurons of the retina, have spatial receptive fields that overlap significantly, leading to correlated firing and redundancy in the visual information that cells encode. Although the strength of correlations among pairs of cells is weak (~10%), the effect in larger populations is dramatic: patterns of spiking and silence in groups of just 10 cells can occur with a probability ~100,000-fold different from that predicted from statistical independence. We show that these strong network correlations can be explained by a model that includes all pairwise interactions, but no higher-order statistics. This model is identical to the Ising model, and predicts that larger populations of neurons may exhibit a form of freezing transition that allows for robust error correction. We have begun to explore these error-correcting properties in simple visual discrimination tasks using large populations of ganglion cells. We find that the correlations among neurons can dramatically reduce the discrimination error.

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3:06PM W7.00002 Exploring the network structure of concerted activity in the primate retina using maximum entropy methods\textsuperscript{1}, JONATHON SHLENS, Salk Institute for Biological Studies — All visual signals in the brain originate in the electrical activity of retinal ganglion cells (RGCs). Standard models implicitly assume that RGCs signal information independently of one another. However, several studies have demonstrated that significant concerted activity in pairs of RGCs may fundamentally alter visual signals. We recorded the electrical activity of several hundred RGCs in peripheral monkey retina. The regular mosaic organization of RGCs that we recorded from nearly every cell in a region of the visual field. In the presence of constant illumination, pairs of RGCs fired synchronously several-fold more often than expected by chance, indicating significant network interactions. Synchrony was localized and universal amongst cells of the same type indicating that it arises from local and highly stereotyped circuitry. To test whether concerted firing can be explained by known pairwise interactions, we used a maximum entropy approach borrowed from statistical mechanics to predict concerted activity. The model accurately reproduced the data. This suggests that network interactions in the primate retina are well approximated by a nearest neighbor Ising model and concerted activity can be understood based on local interactions within a neural population.

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1 NIH grant EY018003; NSF 0333451; NSF PHY-0417175.
A continuous phase transition in neocortical slice networks1. JOHN BEGGS, Indiana University, Bloomington — Recent experiments demonstrate that activity in neocortical circuits can propagate in the form of avalanches whose sizes follow a power law distribution, suggesting that these circuits operate near a continuous phase transition point. Computational models indicate that this critical point may be optimal for information processing. However, the existence of a power law is not sufficient to establish critical behavior because stochastic processes that do not undergo phase transitions can also produce power laws. We recorded power law distributions of neuronal avalanches from neocortical slices and then pharmacologically perturbed network activity. We then measured deviations from power law behavior. Here we show that these deviations covary systematically with a control parameter, as would be expected for a continuous phase transition. A critical branching model captures this transition, while stochastic models do not. Our findings imply that the physical theory underlying continuous phase transitions can be fruitfully applied to neocortical circuits.

Supported by NSF, and MetaCyt funds to Indiana University from Eli Lilly Foundation

4:18PM W7.00004 Patterns of Neural Activity in Networks with Complex Connectivity, SARA A. SULLA, Northwestern University — An understanding of emergent dynamics on complex networks requires investigating the interplay between the intrinsic dynamics of the node elements and the connectivity of the network in which they are embedded. In order to address some of these questions in a specific scenario of relevance to the dynamical states of neural ensembles, we have studied the collective behavior of excitable model neurons in a network with small-world topology. The small-world network has local lattice order, but includes a number of randomly placed connections that may provide connectivity shortcuts. This topology bears a schematic resemblance to the connectivity of the cerebral cortex, in which neurons are most strongly coupled to nearby cells within fifty to a hundred micrometers, but also make projections to cells millimeters away. We find that the dynamics of this small-world network of excitable neurons depend mostly on both the density of shortcuts and the delay associated with neuronal projections. In the regime of low shortcut density, the system exhibits persistent activity in the form of propagating waves, which annihilate upon collision and are spawned anew via the re-injection of activity through shortcut connections. As the density of shortcuts reaches a critical value, the system undergoes a transition to failure. The critical shortcut density results from matching the time associated with a recurrent path through the network to an intrinsic recovery time of the individual neurons. Furthermore, if the delay associated with neuronal interactions is sufficiently long, activity reemerges above the critical density of shortcuts. The activity in this regime exhibits long, chaotic transients composed of noisy, large-amplitude population bursts.

4:54PM W7.00005 Optimal processing and the statistics of visual input signals, ROB DE RUYTER VAN STEVENINCK, Indiana University Bloomington — Sensory information processing can be seen as a statistical estimation problem, where relevant features are extracted from a raw stream of sensory input containing an imperfect representation of those features. Broadly speaking, the optimal solution to the feature extraction problem depends on the statistical structure of those input signals. Here we study the statistics of natural visual input signals, and the optimal solution to the problem of visual motion detection. Motion detection is a biologically important feature estimation problem, as many animals use vision to estimate their motion through space. Many years ago, Reichardt and Poggio drew attention to two important aspects of this problem. First, computing motion from an array of photoreceptors is an irreducibly nonlinear operation, and second, biological versions of this operation seem mathematically tractable. To paraphrase, the problem is interesting but not hopelessly complicated. In this spirit I will discuss motion estimation in the visual system of the blowfly, with an emphasis on performance under natural conditions. As noted above, the array of photoreceptors in the retina implicitly contains data on self motion, but this relation is noisy, indirect and ambiguous due to photon shot noise and optical blurring, and also as a result of the structure of the natural environment. Further, natural variations in the visual signal to noise ratio are enormous, and nonlinear operations are especially susceptible to noise. One can therefore reasonably hope that animals have evolved interesting optimization strategies to deal with large variations in signal quality. I will present experimental data, both from sampling natural probability distributions, and from motion sensitive neurons in the fly brain, that illustrate some of these solutions and that suggest that the fly indeed approaches optimality. The implications of these findings and their possible generalizations will be discussed.

Thursday, March 13, 2008 2:30PM - 5:18PM –
Session W8 DFD: Liquid Crystals II: Dynamics and Topology Morial Convention Center R06

2:30PM W8.00001 Finite element studies of the soft elastic response in liquid crystal elastomers1, BADEL MBANGA, DEREK ARNOSEL, ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ. — When a liquid crystal elastomer film is stretched in a direction transverse to the nematic director, the resulting stress-strain curve typically displays a plateau region, showing a biaxial fluctuations and the possibility of long range tetrahedratic ordering above the nematic phase. Here we report rheological and optical studies on several elastomers that do not undergo phase transitions can also produce power laws. We recorded power law distributions of neuronal avalanches from neocortical slices and then pharmacologically perturbed network activity. We then measured deviations from power law behavior. Here we show that these deviations covary systematically with a control parameter, as would be expected for a continuous phase transition. A critical branching model captures this transition, while stochastic models do not. Our findings imply that the physical theory underlying continuous phase transitions can be fruitfully applied to neocortical circuits.

2:42PM W8.00002 Fluctuating hydrodynamics of nematics for models of liquid-crystal based biosensors via lattice Boltzmann simulations, ORLANDO GUZMAN, JOSE ANTONIO VELEZ, DAVID CASTANEDA, UAM-Iztapalapa — Experimental biosensors based on liquid crystals (LC) use nematics to detect the presence of specific analytes, via the optical textures exhibited by the LC at long times. Efforts to model the time evolution of these textures have relied on relaxation models, ignoring transport phenomena. In this work we include hydrodynamics into a model for these LC biosensors, using lattice Boltzmann (LB) methods and assess the effect on the lifetime of multidomain structures, characteristic of high concentrations of analyte. We apply Yeoman’s et al. LB algorithm, which reproduces the hydrodynamic equations developed by Beris and Edwards for LCs. We also take into account thermal fluctuations, by adding random perturbations to the hydrodynamic modes. Following Adhikari et al., their amplitude is determined by the Fluctuation-Dissipation theorem and we excite both hydrodynamic and the sub-hydrodynamic modes (also called ghost modes). As a result, we analyze the influence of the fluctuations and hydrodynamics on the movement of topological defects.

2:54PM W8.00003 Viscous properties of bent core nematic liquid crystals measured using a nanoliter viscometer1, CHRISTOPHER BAILEY, JOHN HARDEN, ANTAL JAKLI. Kent State University — Since the development of bent core liquid crystal mesogens showing the nematic phase, much work has been done to study the physical properties of these materials in the form of dielectric spectroscopy, dynamic light scattering, and magnetic field induced phase transitions. Some results of these studies showed interesting behaviors such as slow biaxial fluctuations and the possibility of long range tetrahedratic ordering above the nematic phase. Here we report rheological and optical studies on several bent core mesogens showing the nematic and nematic phases. For the rheological studies, we built a viscometer capable of measuring viscoselastic properties with two centipoise resolution with only using 10NL of fluid. Results show abnormal viscosity and optical behavior near the isotropic to nematic phase transition.

1 Acknowledge: Funding provided by NSF-DMR 0606160
3:06PM W8.00004 Electrically induced twist in smectic liquid-crystalline elastomers. Work supported by NSF DMR-0605889 and by ONR.

3:18PM W8.00005 Topography induced homeotropic alignment of nematic liquid crystals.

3:30PM W8.00006 Flexoelectric effect in a bent-core liquid crystal measured by Dynamic Light Scattering.


3:54PM W8.00008 Envelope Dynamics of an Experimental Electroconvection Pattern.

4:06PM W8.00009 Orientational order and topological defects on curved surfaces.

1Supported by NSF DMR-0605889 (R.S. and J.S.), NSF DMR-0426597 (A.T.), and the Institute for Complex Adaptive Matter.
from an ordered state to states with a fixed order parameter (variety of correlated systems. In this talk, we present the results of numerical studies of 2- and 3-dimensional Ising spin systems subjected to thermal cycling.

4:00PM W8.00011 Topology and Geometry of 1D Translational Order on Curved Surface, XIANGJUN XING, SACUCA, State University — It is shown that one dimensional translational order on two dimensional curved substrate is naturally described by differential forms. A new type of global dislocation defects is identified and its relation with the topological properties of the embedding (compact) manifold is explored using algebraic topological methods. The associated topological charge classifies all ground states with no local defects. The energetics of smectic order on curved substrate is also discussed. Coupling between nematic director field and extrinsic curvature is shown to be important. As a simple application, the phase diagram of smectic order on a torus is analyzed. Two phases are identified: a small/thin phase where the nematic director is locked by curvature and a large/fat phase where the director varies continuously with system parameters.

4:18PM W8.00010 Local photo-reorientation of a liquid crystal using a laser focused on an azo-dye-based monolayer, YUE SHI, NOEL CLARK, Department of Physics and Liquid Crystal Material Research Center, University of Colorado at Boulder — The orientation adopted by molecules in an azobenzene-based self-assembled monolayer (azo-SAM) is perpendicular to the polarization of incident green light due to isomerization, aligning liquid crystal (LC) correspondingly. To study the local photo reorientation of the LC, the exciting laser is focused into a small spot on the azo-SAM, of a hybrid cell made with nematic LC sandwiched between the azo-SAM and a homeotropic surface. Under irradiation with changing polarization, a variety of interesting phenomena are observed, including winding of rings of reorientation and orientational slipping. Results vs. exciting light intensities and different rotating frequencies will be reported.

4:30PM W8.00011 Topology and Geometry of 1D Translational Order on Curved Surface, XIANGJUN XING, SACUCA, State University — It is shown that one dimensional translational order on two dimensional curved substrate is naturally described by differential forms. A new type of global dislocation defects is identified and its relation with the topological properties of the embedding (compact) manifold is explored using algebraic topological methods. The associated topological charge classifies all ground states with no local defects. The energetics of smectic order on curved substrate is also discussed. Coupling between nematic director field and extrinsic curvature is shown to be important. As a simple application, the phase diagram of smectic order on a torus is analyzed. Two phases are identified: a small/thin phase where the nematic director is locked by curvature and a large/fat phase where the director varies continuously with system parameters.

4:42PM W8.00012 Coarsening of two-dimensional islands in freely suspended smectic A films, DUONG NGUYEN, CHEOL PARK, JOSEPH MACLENAN, MATTHEW GLASER, NOEL CLARK, University of Colorado, Boulder — We have observed coalescence driven coarsening of islands (edge dilation loops) in freely suspended Smectic A liquid crystal films. This is a good realization of a two-dimensional system, with films as thin as one molecular length (3-4 nm). The film is drawn by spreading material across a circular hole of about 4 mm in diameter, after which the film is suspended by the meniscus in contact with the edge of the hole. Islands are generated by blowing air parallel to the film surface, which produces a shearing force that breaks a thick region of the film into circular islands. Depending on the Smectic A material, we observe either strong or weak short-range repulsion between dilation loops, leading to slow or fast coalescence, respectively. Over time, the average size of islands increases as the number of islands drops. The observed coarsening dynamics is compared with theoretical predictions.

4:54PM W8.00013 The Ground States of Nematic Order on a Sphere and Topological Defects, HOMIN SHIN, MARK BOVICK, XIANGJUN XING, SACUCA, State University — We study the ground states of a spherical nematic order and the resulting configuration of topological defects. To emulate the ground state, we use hard rods confined on the surface of a sphere and very gradually compress the system up to the maximum packing density with Monte Carlo simulations. The nematic phases with four +1/2 disclination defects are clearly observed. Although the tetrahedral structure of four +1/2 defects is expected, we find all the defects most likely sitting on a great circle. The theoretical reasoning is provided with the calculation of defect energies in terms of the elastic anisotropy. Finally, we present that the allowance of some softness to the rods gives rise to qualitative changes in the director field surrounding the defect core.

5:06PM W8.00014 Thermal-Cycle Memory Functions and Ising Dynamics, BRAD JOHNSON, DAVID PATRICK, Advanced Materials Science and Engineering Center, Western Washington University — The Ising model provides a rich system for the study of a variety of correlated systems. In this talk, we present the results of numerical studies of 2- and 3-dimensional Ising spin systems subjected to thermal cycling from an ordered state to states with a fixed order parameter (<1), with differing overall morphologies, and back to a quenched state. We find that for systems with initial states generated by thermal disordering above Tc, the initial state of a given order parameter has larger ‘islands’ of like-spin (than the case for random disorder with the same overall order parameter) and consequent quenches of the state to T<Tc result in a strong correlation to a particular final average order parameter. The function we find is given by (S) ≈ tanh(B + Sinit), where Sinit is the order parameter of the initial state, <S> is the average quenched order parameter, and B is a constant that depends upon the morphology of the initial state. The reason for the strong correlation stems from the energies associated with spins at the borders of large clusters. This ‘memory effect’ does not occur in 3D (due to the larger number of near-neighbors). Finally, we discuss the ‘memory function’ in the context of interfacial states of liquid crystals.

Thursday, March 13, 2008 2:30PM - 5:30PM — Session W9 DCMP: Theoretical Methods and Applications Morial Convention Center R07

2:30PM W9.00001 Polarization model revisited, MICHAEL GALPERIN, Los Alamos National Laboratory, ABRAHAM NITZAN, Tel Aviv University, MARK A. RATNER, Northwestern University — We revisit a polaron model proposed by us as a possible mechanism for nonlinear conductance, and discuss difference in polaron formation within isolated system vs. molecular junction situation. Within one-level model we present approximate expression for electronic Green function corresponding to inelastic transport case, which in appropriate limits reduces to expressions presented previously for isolated molecule and for molecular junction coupled to slow vibration (static limit). Relevance of the isolated molecule-type consideration to describe properties of molecular junctions is discussed.

2:42PM W9.00002 A theoretical investigation of the porphyrin-gold junction: applications to molecular wires, MATT MCKENZIE, ZORABEL LEJEUNE, JAYNE GARNO, BING CHEN, Louisiana State University — An important step in the miniaturization of electronic devices involves molecular wires and junctions at the nanoscale level. Porphyrins are a promising material for such objects because of their unique electronic, chemical, and optical properties. The model porphyrin used in this study is a free based tetra-substituted with two phenyl rings and two pyridyl rings as peripheral groups which could provide a mechanism for enhanced electron transfer. The goal of this study is to elucidate the electron transfer processes between the model porphyrins and Au(111). The orbital structures and properties are determined using Car-Parrinello molecular dynamics. The geometry of the porphyrin on the gold surface is explored; from a complete reorientation of the molecule with respect to the surface to different orientations of the pyridyl groups. The calculated electronic conductivity, using the Kubo-Greenwood formula, will be compared to experimental findings using conductive probe Atomic Force Microscopy.
2:54PM W9.00003 Ion-Ion Interactions in Simple Metallic Systems: Beyond Linear Response

JAMES PORTER, Dept. of Physics and Astronomy, Colby College, NEIL ASHCROFT, GEOFFRÉY CHESTER, Laboratory of Atomic and Solid State Physics, Cornell University — We extend the formalism of electronic response theory to second order in perturbing pseudopotentials and examine the physical consequences on effective ionic pair potentials for certain simple metals, under standard conditions. The pseudopotentials, assumed to be transferable, are of the Ashcroft empty-core form. Our results show that inclusion of second-order response terms in the pair potentials leads to the deepest potential minima having locations that are within 8% of the experimental nearest neighbor distances for crystalline sodium, magnesium, aluminum, and metallic silicon, all in their standard one-atom atmospheres. Second-order response effects are found to be becoming increasingly important as the valence increases. We briefly discuss two natural extensions of this research, namely to three-body potentials and to changes expected in pair potentials at higher densities.

1 This work was supported by the National Science Foundation.

3:06PM W9.00004 Algorithm for extraction of quantum oscillation orbits from band structure data

PATRICK ROURKE, STEPHEN JULIAN, University of Toronto — In determining the Fermi surface of a material, quantum oscillation measurements are often compared to band structure calculations. Each oscillation frequency corresponds to an electron (or hole) orbit on the Fermi surface, perpendicular to the applied magnetic field; only orbits enclosing areas that are locally extremal are detected. To facilitate comparisons between theory and experiment, we have developed an algorithm, "SKGAEF," which finds extremal orbits in band structure calculations and determines quantum oscillation frequencies, effective masses and band specific heat contributions. Our code uses a k-space supercell approach, and can successfully locate geometrically-complicated orbits. Example results will be presented for the heavy fermion material UPt3.

3:18PM W9.00005 Development of the relativistic tight-binding model for Platinum

ALEXANDER TCHERNATINSKY, J. WOODS HALLEY, University of Minnesota — As a first step in a program to understand the mechanism of oxygen reduction on a platinum surface in an aqueous environment, we developed a relativistic self consistent tight- binding model for platinum. We applied a scheme that we successfully previously used for the description of titanium (S. Erdin, et al., PRB, 72, 035405 (2005)) in which the electronic structure problem is described by an energy functional containing onsite terms depending self consistently on the local charge and interatomic terms. Due to the high atomic number of platinum, relativistic effects are known to be significant in the electronic structure. We include relativistic effects in the onsite functions of the tight binding model by making them self consistently dependent on the local Mulliken charge (as before) and also on the expectation values of the total atomic angular momentum number $J$ of the atom and the occupation numbers of the $5d_{3/2}$ and $5d_{5/2}$ atomic orbitals in the tight binding basis. We find that this set of variables can uniquely describe the low energy states of the isolated platinum atom including relativistic effects. Their values are calculated self consistently in the tight binding model for the metal. The model was used to calculate the electronic structure of relaxed, low index platinum surfaces. Results will be compared with DFT results and with experiment. This work was supported in part by Minnesota Supercomputing Institute and U.S.DOE.

3:30PM W9.00006 Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations

LIPING YU, V. RANJAN, NC State U, Raleigh, W. LU, J. BERNHOLC, M. BUONGIORNO NARDELLI, NC State U, Raleigh and ORNL, TN — In ab initio calculations for surfaces or non-periodic systems one often relies on the supercell approximation, where periodic replicas are separated by enough empty space to avoid spurious interactions between successive images. However, a vacuum separation is not sufficient to screen dipolar interactions that appear in asymmetrically charged or polar systems. Two solutions have been proposed in the literature: (i) the dipole correction, and (ii) Coulomb cutoff formalism that eliminates interactions between periodic replicas. We compare these methods under the same conditions in the framework of plane wave DFT calculations. It is found that the two methods produce equivalent results for the total energy, force, charge density and self-consistent potential. In band structure calculations, the results coincide for occupied states but differ for delocalized unoccupied ones in small supercells. This discrepancy can be used as a criterion to identify supercell sizes that are sufficiently large to obtain converged results.

3:42PM W9.00007 Issues related to Convergence Properties of First Principles Full Potential Multiple Scattering Electronic Structure Calculations

AURELIAN RUSANU, G. MALCOLM STOCKS, MARKUS EISENBACK, DON M. NICHOLSON, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputer Center — Despite some clear advantages for specific problems, the implementation of full potential electronic structure methods based on the use of multiple scattering theory (MST) (KKR derived approaches) has received much less investment than alternate electronic structure methods. Here we describe some new techniques that facilitate an easy and accurate implementation of first principles full potential MST methods. The method consists of solving: (1) the full-potential single site scattering problem, where we avoid the usage of the shape function by surface integrals methods to determine the scattering matrices, and (2) the Poisson problem, where the site centered full-potential is constructed from a sphere bounded non-overlapping charge density and a smooth space-filling charge density. Specifically, we discuss issues related to accuracy and convergence properties of these techniques within the context of the order-N Locally Self-consistent Multiple Scattering (LSMS) method.

1 Work supported by US-DOE, Office of Basic Energy, Division of Materials Science and Engineering.

3:54PM W9.00008 First-principles investigation of electronic band gap in multiwalled carbon nanotube: Role of mechanical deformations

PAVAN K. VALAVALA, Department of Physics and Mechanical Engineering-Engineering Mechanics, Michigan Technological University, GREGORY M. ODEGARD, Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, RANJIT PATI, Department of Physics, Michigan Technological University, Houghton, MI 49931 — The carbon nanotube (CNT) structures have been the subject of intense research in recent years. Some studies have shown that the electronic band gap in single walled CNT can be modulated through mechanical deformations such as flattening. It has been shown that single walled CNTs undergo a semiconductor-metallic and semiconductor-metallic-semiconducting transition when subjected to deformations. However, the modulation of electronic band gap of multiwalled CNT under mechanical deformations has not been studied. We have used first- principles gradient density functional approach to explore the role of flattening on the electronic properties of MWCNT structures. The influence and the effect of flattening on the electronic properties of the constituent single walled CNTs are also explored.

4:06PM W9.00009 Atomic-scale Analysis of the Interactions Between Atomic Hydrogen and Multi-walled Carbon Nanotubes

ANDRE R. MUNIZ, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts at Amherst — We present a detailed atomic-scale analysis of the interactions of atomic hydrogen with the internal layers of multi-walled carbon nanotubes (MWCNTs). The analysis is based on a synergistic combination of classical molecular dynamics (MD) with first-principles density functional theory (DFT). The Adaptive Interatomic Reactive Empirical Bond Order (AIREBO) potential is employed in the MD simulations of H-MWCNT interactions and the resulting structural relaxations. Parameters that have been varied in our analysis include nanotube diameters, number of nanotube walls, inter-wall spacing, and temperature. The MD simulations reveal that, under certain conditions, H chemisorption onto internal MWCNT walls and H diffusion in the space between walls can induce the formation of inter-shell sp3 C-C bonds. The MD mechanisms are in good agreement with our DFT calculations of optimal pathways of C-C bond formation and provide interpretations for the formation of nanocrystalline carbon, which has been observed experimentally upon H2 plasma exposure of MWCNTs.
4:18PM W9.00010 Electronic Property Control of Single-Walled Carbon Nanotubes by Functionalization. CHIAYUN WU, YOUNG-KYUN KWON, Univ of Mass - Lowell — Single-walled carbon nanotubes exhibit remarkable electronic properties. It is well known that there are two types of single-walled carbon nanotubes: metallic and semiconducting. However, separating semiconducting carbon nanotubes from metallic ones is a “holy grail” problem in nanoelectronics fields. Using ab initio density functional theory, we will present the effects of various functional groups, such as 4-bromobenzene diazonium tetrafluoroborate, on SWNTs. Modifications in electronic and transport properties due to such functionalization will be discussed. Possible mechanism converting metallic tubes to semiconducting ones will be addressed.

4:30PM W9.00011 Design of Janus Nanoparticles with Atomic Precision. QIANG SUN, Peking University, QIAN WANG, PURU JENA, Virginia Commonwealth University, YOSHI KAWAZOE, Tohoku University — Janus nanoparticles, characterized by their anisotropic structure and interactions have added a new dimension to nanoscience because of their potential applications in biomedicine, sensors, catalysis and assembled materials. The technological applications of these nanoparticles, however, have been limited as the current chemical, physical, and biosynthetic methods lack sufficient size and shape selectivity. We report a technique where gold clusters doped with tungsten can serve as a seed that facilitates the natural growth of anisotropic nanostructures whose size and shape can be controlled with atomic precision. Using ab initio simulated annealing and molecular dynamics calculations on Au\_nW (n>12) clusters, we discovered that the W\_n@Au\_12 cage cluster forms a very stable core with the remaining Au atoms forming patchy structures on its surface. The anisotropic geometry gives rise to anisotropies in vibrational spectra, charge distributions, electronic structures, and reactivity, thus making it useful to have dual functionalities. In particular, the core-patch structure is shown to possess a hydrophilic head and a hydrophobic tail. The W\_n@Au\_12 clusters can also be used as building blocks of a nano-ring with novel properties.

4:42PM W9.00012 Uniaxial compression of group-IV nanoparticles from ab-initio molecular dynamics simulations. PRASANJIT SAMAL, MATTEO COCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 - 0132, U.S.A. — Uniaxial compressions of isolated systems from ab-initio molecular dynamics are made possible through the extension of the electronic enthalphy method [Phys. Rev. Lett. 94, 145501 (2005)] previously introduced for finite systems under hydrostatic pressure. Through this novel approach experimental settings with nanoparticles indented between parallel plates can be reproduced and simulated more realistically, thus allowing for more reliable comparisons between experimental data and simulation results. Molecular dynamics simulations for some group-IV nanoparticles under uniaxial compression have been performed using this extended scheme. Comparison with the deformation of the same systems under hydrostatic loads will elucidate the differences and similarities in the nucleation events of structural transformations and in their kinetic pathways.

4:54PM W9.00013 Explaining the electroluminescence of single molecules. JOHN BUKER, GEORGE KIRCZENOW, Simon Fraser University — Experimental studies of electroluminescence from molecules on complex substrates have yielded intriguing relationships between the current-voltage characteristics and optical emission from such systems. In this talk we propose a theoretical model that is able to account for many observed properties of these systems. We obtain distinct photon emission spectra and corresponding I-V curves for different couplings of the electrodes to the molecule, that are consistent with experimental data. We find emission to be highly dependent on the details of the tip/molecule and molecule/substrate coupling, and make further photon emission predictions for systems not yet achieved experimentally.

5:06PM W9.00014 Toward quantitative acoustic molecular gas sensing. ANDI PETCULESCU, University of Louisiana at Lafayette — Laser spectroscopy techniques provide unrivaled tools for detailed molecular sensing studies. Critical applications such as gas monitoring in life-support systems often require sensors that are not only fast and sufficiently accurate but also rugged and not needing extensive maintenance and calibration. Acoustic sensors are widely used to this end, based on measuring sound speed changes. These, however, can only constrain the overall molecular mass. For reasons unknown, researchers have habitually disregarded acoustic attenuation. Beside the classical sound loss mechanisms due to viscosity, heat conduction, and diffusion, the non-classical contribution to attenuation arises from the inability of internal molecular degrees of freedom to follow the acoustic temperature fluctuations. This connects acoustic attenuation to the molecular relaxation times. In the laboratory, acoustic studies of molecular relaxation in fluids require that the ambient pressure be varied over a wide range at a given frequency in order to cover the relaxation processes. In a fast-sensing device, this would be highly impractical. A novel algorithm is presented here relying on measuring sound speed and attenuation at one pressure and two frequencies to reconstruct the full frequency dependence of the effective specific heat for the main relaxation processes. This would enable a smart sensor to infer the concentration and nature of contaminant molecules in a base gas.

5:18PM W9.00015 A delta-function model for three-dimensional axisymmetric crystals. PING DU, HARRIS WONG, Louisiana State University — A surface energy polar plot contains two possible singularities: the cusps that give facets on an equilibrium crystal, and the circular arcs connecting the cusps that can lead to missing orientations. The common approach of specifying the surface energy usually cannot handle both singularities simultaneously. We model the surface stiffness to avoid missing orientations. Furthermore, a facet is represented by the Dirac delta function with the weight of the delta function equal to the width of the facet. Thus, both singularities are treated precisely. This approach has been shown to work for two-dimensional symmetric [1] and axially symmetric [2] crystals. Here, we apply the delta function to model three-dimensional axisymmetric crystals and obtain analytic solutions to the nonlinear differential equation governing the crystal shape. We find that at every point on the crystal surface the chemical potential is equipartitioned between the axial and the azimuthal component.


Thursday, March 13, 2008 2:30PM - 5:18PM
Session W10 DMP: Focus Session: Hybrid Magnetic-Superconducting Systems III Morial Convention Center RO8
through transport measurements, both for bulk and mesoscopic samples. This work was supported by FWO-Vl, IUAP and BOF/UA (Belgium) and CNPq (Brazil), FAPERJ (Brazil), FAPERJ (Brazil), and the National Science Foundation (US) through grant ECS-0202780 and by DOE under contract No. DE-AC-02-06CH11357.

3:30PM W10.00004 Vortex lattice matching effects in superconducting Mo₃Si films with magnetic pinning centers. , DAVID PEREZ DE LARA, Dept. Fisica de Materiales, Universidad Complutense, 28040 Madrid (Spain), ALEJANDRO ALIJA, ALEJANDRO JUNQUERA, Dept. Fisica, Universidad Oviedo, 33007 Oviedo (Spain), JOSE M. COLINO, Dept. de Fisica, Universidad de Castilla la Mancha, Ciudad Real, Spain, JESUS MARTIN, Dept. Fisica de Materiales, Universidad Complutense, 28040 Madrid (Spain), MARIA VELEZ, Dept. Fisica, Universidad Oviedo, 33007 Oviedo (Spain), JOSE V. ANGUITA, Instituto Microelectronica, CSIC, Tres Cantos, 28760, JOSE L. VICENT, Dept. Fisica de Materiales, Universidad Complutense, 28040 Madrid (Spain) — Electron Beam Lithography and sputtering techniques have been used to fabricate arrays of Ni nanodots on Si (100) substrate. Nb films and amorphous Mo₃Si films were grown on top of the magnetic array by magnetron sputtering. The same arrays were used in both superconducting systems; therefore the same periodic pinning potential is induced in both systems. Magnetotransport and (I, V) curves were measured close to the films critical temperatures. Matching effects are observed between the periodic array of pinning potentials and the driving vortex lattice. The different vortex dynamics will be discussed in both systems. We want to thank Spanish Ministerio de Educacion y Ciencia grants NAN2004-09087, FIS2005-07392.

3:42PM W10.00005 Confined vortex phase in superconductor-ferromagnet nanocomposites. , MILORAD MILOSEVIC, Departement Fysica, Universiteit Antwerpen, Belgium, MAURO DORIA, Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil, FRANCISCO PEEGERS, Departement Fysica, Universiteit Antwerpen, Belgium — In the fifties, Abrikosov found the coexistence of superconductivity with magnetic vortices in the superconducting density of states in the coexistence region is followed as function of temperature and external magnetic field. Similar to exotic superconductors, internal complexes of vortex loops may also arise around embedded nanomagnets in artificial superconducting hybrids, where high density of magnetic particles can be controlled by tuning the strength of the field emanating from the dots and compensating the applied field. Static vortex patterns and dynamic effects, such as guided vortex motion and vortex ratchet effects, were studied in the superconductor/ferromagnet hybrids consisting of the superconducting film covered by magnetic dots, bars, loops with the in-plane magnetization. In-plane magnetic dipoles create asymmetric pinning sites responsible for the appearance of the magnetic dipole vortex ratchets theoretically predicted by Carneiro and now found experimentally. Switchable flux pinning landscape has been created by tuning the magnetic states of the in-plane magnetized loops. (Phys.Rev.Lett. 98, 117005 (2007), Appl. Phys. Lett. 90, 182501 (2007), Phys. Rev. B (R) 76, 60503 (2007))

4:30PM W10.00006 Interplay of Superconducting with Magnetic Vortices, A. HOFFMANN, J.E. PEARSON, G. MIHAJLOVIČ, MGD and CNM, Argonne National Laboratory, V. METLUSHKO, L. FUMAGALLI, J.C. SAUTNER, N. JAHEDI, ECE, University of Illinois at Chicago, — Periodic arrays of magnetic structures are well known to give rise to commensurate pinning of superconducting vortices in adjacent superconducting films. We compared the pinning effects due to magnetic dots with either single domain or vortex magnetization configuration. There is a clear correlation between the magnetoresistance in the superconductor and the magnetization configuration of the magnetic dots, indicating that the pinning of the superconducting vortices is strongly enhanced for the magnetic vortex state. The origin of this enhanced pinning is due to the locally larger magnetic stray fields produced by the magnetic vortex cores. The absence of an symmetry for parallel and anti-parallel orientation between the superconducting vortex flux and the magnetic vortex cores suggests that the enhanced pinning is not due to magnetostatic interactions but is rather due to the local suppression of superconductivity by highly localized, large perpendicular stray magnetic fields generated by the magnetic vortex cores.
4:06PM W10.00007 Enhancement of superconductivity by parallel magnetic field in ultrathin α-Pb films. ASHWANI KUMAR, H. JEFFREY GARDNER, PENG XIONG, Department of Physics and MARTECH, Florida State University — A modified dilution refrigerator equipped with in situ film growth and a rotating sample stage is used to study the effect of magnetic field on ultrathin homogeneous Pb films. An insulating layer of Sb (~ 1 nm) is first deposited to ensure electrical and possibly structural uniformity down to a single atomic layer for the subsequently deposited Pb. Through incremental deposition of Pb, a film with increasing thickness (thus decreasing R and increasing Tc) is obtained and transport measurements in perpendicular and parallel magnetic field are performed in situ at different film thicknesses. Any perpendicular field is found to suppress superconductivity, and at sufficient strength induces an electrically inhomogeneous insulating state. In contrast, the same film is at least two orders of magnitude less sensitive to a parallel field. More strikingly, a moderate parallel magnetic field actually increases the Tc of the film, resulting in large negative magnetoresistance in the transition region in parallel fields as large as 3T. The dependence of this effect on the film thickness, impurities and temperature will be presented and discussed. 1J.S. Parker et al., Europhys. Lett. 75, 950 (2006).

4:18PM W10.00008 An Effective Action approach to inhomogeneous superconductors: Application to F/S/F spin valves. ADNAN REBEI, Seagate Technology — The interplay between magnetism and superconductivity can be studied in simple systems such as ferromagnetic-superconductor-ferromagnetic tri-layers. Many recent experiments [1] measured a critical temperature dependence of the superconductor as a function of the relative orientations of the surrounding ferromagnetic layers. This layered system gives rise to an in-homogenous gap equation for the superconductor due to the polarization at the ferromagnetic-superconductor interfaces irrespective of the orientation of the magnetization in-plane or out-of-plane. Real space formulations are therefore better suited to study this kind of systems. We show that an Effective Action formulation similar to the one proposed by Weinberg [2] is very advantageous in this respect as was shown in normal-ferromagnetic-normal systems in [3].


4:30PM W10.00009 Multilayered ferromagnet/superconductor nanostructures: proximity effect, decoupled superconductivity, and hierarchy of critical temperatures. Y. N. PROSHIN, Kazan State University, Russia, N. G. FAZLEEVA, University of Texas at Arlington, USA, M. G. KHUSAINOV, Vostok branch, Kazan State Technical University, Russia — The four-layered F'/S'/F''/S'' nanostructure consisting of rather dirty superconducting (S) and ferromagnetic (F) metals is studied within the theory of the proximity effect taking detailed account of the boundary conditions. The new pi phase superconducting states are obtained for the F'/S'/F''/S'' nanostructure in addition to the known “superlattice” states. The dependence of the critical temperature versus the F layers thicknesses is investigated. It is shown that the F'/S'/F''/S'' nanostructure can experience decoupled superconductivity. The latter manifests itself through a hierarchy of the critical temperature Tc, which can be different for different S' and S'' layers. An optimal set of parameters is determined, for which the difference between the critical temperatures for different S' and S'' layers becomes significant. The corresponding phase diagrams are constructed and discussed.

4:42PM W10.00010 Paramagnetic Intrinsic Meissner Effect in Layered Superconductors\(^1\). ANDREI LEBED, Dept. of Physics, University of Arizona — Free energy of a quasi-two-dimensional superconductor with a coherence length perpendicular to the conducting layers being less than an inter-layer distance is calculated. The free energy is shown to differ from that in the textbook Lawrence-Doniach model at high fields, where the Meissner currents are found to create an unexpected positive magnetic moment due to shrinking of the Cooper pairs “sizes” by a magnetic field. This unique phenomenon - paramagnetic intrinsic Meissner effect (PIME) in a bulk [1] - is suggested to detect by measuring in-plane magnetization and torque in layered organic and high-Tc superconductors as well as in superconducting superlattices.


\(^1\)This work is supported by the NSF grant DMR-0705986.

5:06PM W10.00012 Synchronization by internal cavity mode and resonant electromagnetic emission from intrinsic Josephson junction stacks\(^1\). ALEXEI KOSHELEV\(^2\), Argonne National Laboratory — Intrinsic Josephson-junction stacks realized in mesas fabricated out of high-Tc superconductors may be used as sources of coherent electromagnetic radiation. The major challenge is to synchronize Josephson oscillations in all junctions to get significant radiation. A simple way to solve this problem is to excite the in-phase Fiske mode when the Josephson frequency matches the Fiske-resonance frequency set by the stack lateral size[1]. A finite direct coupling to such mode exists in mesas with lateral modulation of the Josephson critical current identical in all junctions [2]. The powerful almost standing electromagnetic wave is excited inside the crystal in the resonance promoting full synchronization. We evaluate behavior of the I-V characteristics and radiated power near the resonance. We will discuss several relevant issues including (i) stability of the coherent state, (ii) mechanism of damping including external radiation and leaking of radiation into the bulk crystal, and (iii) angular dependence of external radiation. [1] L. Ozyuzer, et al. Science 318, 1291 (2007) [2] A. E. Koshelev and L. N. Bulaevskii, cond-mat 0708.3269

\(^1\)This works was supported by the Department of Energy under contract No. DE-AC02-06CH11357

\(^2\)and Lev Bulaevskii (LANL)

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Thursday, March 13, 2008 2:30PM - 5:18PM –
Session W11 DCMP: Theory of Superconductivity in Cuprates II Morial Convention Center R09
2:30PM W11.00001 Theory of Strongly Correlated Superconductivity[^1]. WILLIAM PUTIKKA, Ohio State University — Superfluid behavior is relatively common in strongly correlated fermion systems. This suggests there is a common reason for this behavior rooted in the strong correlations. I propose such a mechanism, developed in the context of the 2D $t$-$J$ model, where $d_{x^2-y^2}$ superconducting fluctuations have recently been observed[^1]. The $d_{x^2-y^2}$ fluctuations are not due to antiferromagnetic spin fluctuations; the AF fluctuations compete with superconducting fluctuations. Pairing fluctuations have their own origin based on strong correlations. The key to understanding how this comes about is the high temperature entropy. Strong correlations not only create order at low temperatures, they also reduce the entropy at high temperatures. The response of the system is to rearrange the degrees of freedom into separate spin and charge excitations. These excitations have very different energy scales, allowing the charges to develop pairing correlations before the spin degrees of freedom become coherent. At lower temperatures where the spins become coherent they determine the symmetry of the electronic pairing wavefunction in a manner to best avoid the magnetic fluctuations in the system.

[^1]: Supported by NSF ECS-0523918.

2:42PM W11.00002 Magnetism and superconductivity in the $t$-$t'$-$J$ model. FEDERICO BECCA, LEONARDO SPANU, MASSIMO LUGAS, SANDRO SORELLA, CNR-INFM Democritos and SISSI (Trieste) — We present a systematic study of the phase diagram of the $t$-$t'$-$J$ model by using the Green's function Monte Carlo (GFMC) technique, implemented within the fixed-node (FN) approximation and a wave function that contains both antiferromagnetism and d-wave pairing. This enables us to study the interplay between these two kinds of order and compare the GFMC results with the ones obtained by the simple variational approach. By using a generalization of the forward-walking technique, we are able to calculate true FN ground-state expectation values of the pair-pair correlation functions. In the case of $t' = 0$, there is a large region with a coexistence of superconductivity and antiferromagnetism, that survives up to $\delta_c \sim 0.10$ for $J/t = 0.2$ and $\delta_c \sim 0.13$ for $J/t = 0.4$. The presence of a finite $t'/t < 0$ induces a strong suppression of both magnetic (with $\delta_c < 0.03$, for $J/t = 0.2$ and $t'/t = -0.2$) and pairing correlations. In particular, the latter ones are depressed both in the low-doping regime and around $\delta \sim 0.25$, where strong size effects are present.

2:54PM W11.00003 Phase Fluctuations in high-Tc Superconductors. YUCEL YILDIRIM, WEIGUO YIN, WEI KU, Brookhaven National Laboratory — Thermal fluctuation induced destruction of phase coherence of superconductivity in High-Tc superconductors is investigated via numerical quantum Monte Carlo solution of a new theoretical model at finite-temperature. Our simple effective boson Hamiltonian, derived from the pairing sector of the $t$-$t'$-$J$ model, can be considered as a natural extension of the hard-core boson with additional information about the internal structure of the local fermion pairs. The local solution is found to consist of d-wave pairing, hybridizing with neighboring p-wave pairs. The possible connection with the pseudo-gap phase will also be addressed.

3:06PM W11.00004 Suppression of Superfluid Density in Underdoped Cuprates. WEI-CHENG LEE, Department of Physics, the University of Texas at Austin, Austin TX 78712, JAIRAINO SINNOVA, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA, ANTON O. BURKOV, Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1, YOGESH JOGLEKAR, Department of Physics, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana 46202, USA, ALLAN H. MACDONALD, Department of Physics, the University of Texas at Austin, Austin TX 78712 — A key challenge for theories of high-$T_c$ cuprates is to explain why the superfluid density vanishes as the antiferromagnetic insulator state is approached. Viewing a cuprate as a doped Mott insulator gives a natural explanation for this property, but one that is not obviously compatible with the fact that superconductivity always vanishes at finite doping. We propose another possible explanation, starting from weak-coupling conventional d-wave BCS theory and calculating the correlation contribution to the superfluid density. We show that triplet fluctuations of the d-wave superconducting order parameter are canonically conjugate to antiferromagnetic fluctuations, and that this causes the correlation energy to increase in magnitude when superconductivity is weakened by a phase gradient. In our theory the inelastic neutron scattering resonance has the character of a magnetic plasmon rather than the character of an exciton.

3:18PM W11.00005 Stability of inhomogeneous superconducting states in the doped t-J model. MANUELA CAPELLO, DIDIER POILBLANC, Laboratoire de Physique Theorique, CNRS, and Universite Paul Sabatier, Toulouse, France — Using quantum Monte Carlo techniques, we have investigated the stability of inhomogeneous RVB superconducting states in the $t$-$J$ model by using the Green's function Monte Carlo (GFMC) technique, implemented within the fixed-node (FN) approximation and a wave function that contains both antiferromagnetism and d-wave pairing. This enables us to study the interplay between these two kinds of order and compare the GFMC results with the ones obtained by the simple variational approach. By using a generalization of the forward-walking technique, we are able to calculate true FN ground-state expectation values of the pair-pair correlation functions. In the case of $t' = 0$, there is a large region with a coexistence of superconductivity and antiferromagnetism, that survives up to $\delta_c \sim 0.10$ for $J/t = 0.2$ and $\delta_c \sim 0.13$ for $J/t = 0.4$. The presence of a finite $t'/t < 0$ induces a strong suppression of both magnetic (with $\delta_c < 0.03$, for $J/t = 0.2$ and $t'/t = -0.2$) and pairing correlations. In particular, the latter ones are depressed both in the low-doping regime and around $\delta \sim 0.25$, where strong size effects are present.

3:30PM W11.00006 “Glue” approximation for the pairing interaction in the Hubbard model with next nearest neighbor hopping. EHSAN KHATAMI, ALEXANDRU MACRIDIN, MARK JARRELL, University of Cincinnati — Recently, several authors have employed the “glue” approximation for the Cuprates in which the full pairing vertex is approximated by the spin susceptibility. We study this approximation using Quantum Monte Carlo Dynamical Cluster Approximation methods on a 2D Hubbard model. By considering a reasonable finite value for the next nearest neighbor hopping, we find that this “glue” approximation, in the current form, does not capture the correct pairing symmetry. Here, d-wave is not the leading pairing symmetry while it is the dominant symmetry using the “exact” QMC results. We argue that the sensitivity of this approximation to the band structure changes leads to this inconsistency and that this form of interaction may not be the appropriate description of the pairing mechanism in Cuprates. We suggest improvements to this approximation which help to capture the the essential features of the QMC data.

3:42PM W11.00007 Pairing glue in the Hubbard and t-J models: Insights from a dynamic cluster approximation study. THOMAS MAIER, Oak Ridge National Laboratory, DOUGLAS SCALAPINO, University of California, Santa Barbara, MARK JARRELL, University of Cincinnati — We will discuss dynamic cluster non-crossing approximation studies of the superconducting gap function $\Phi(k,\omega)$ in the 2D Hubbard and t-J models. The momentum and frequency dependence of the gap reflect the spatial structure and dynamics of the pairing interaction responsible for d-wave pairing. For both models we find that two mechanisms are simultaneously active. An instantaneous contribution to the gap arises from states whose energies reflect the Mott scale and which give rise to the exchange coupling $J$. The dominant contribution, however, is retarded and comes from energies that correspond to the spin fluctuation spectrum. It is therefore reasonable to speak of a dynamic “pairing glue” which gives rise to d-wave superconductivity in the Hubbard and t-J models.
Arizona — The superconducting $\kappa$ explained within an anisotropic triangular lattice\[1\] under ambient pressure, and the appearance of superconductivity under pressure has led several investigators to suggest that the superconductivity can be , HONGTAO LI, University of Arizona, R. TORSTEN CLAY, Mississippi State University, S. MAZUMDAR, University of A triangular lattice observed in transport measurements at the special structure of La $\text{Ba}_2\text{Cu}_3\text{O}_6$.\[1\] $\text{CuO}_2$.

We speculate that this effect could lead to a region of globally phase coherent portion of the superconducting order must have s-wave symmetry. We find that the Josephson coupling between the s-wave components of the order parameter on two droplets separated by a distance $r$ falls off as a slower power law than does the d-wave component. Thus, for dilute enough droplets, even if the local gap structure within each droplet is dominantly d-wave-like, we do not find any hint of long range superconducting correlations. Neither is there any region of the Hubbard $d$ limit, when antiferromagnetism gives way to d-wave superconductivity. We have performed exact diagonalizations on a 16-site periodic anisotropic triangular electronic system, under a set of special circumstances, the superconducting condensate, like the magnetic order, can occur at a nonzero wave vector corresponding to a spatial period double that of the charge order. In this case, the Josephson coupling between near neighbor planes, especially in a crystal with the special structure of $\text{La}_2\text{Ba}_2\text{Cu}_3\text{O}_6$, vanishes identically. We propose that this is the underlying cause of the dynamical decoupling of the layers recently observed in transport measurements at $x = 1/8$.

Many experimental implications of various types of assumed order are discussed in the context of the cuprate superconductors.

Disorder

Some experimental implications of various types of assumed order are discussed in the context of the cuprate superconductors.

Disorder

4:06PM W11.00009 Dynamical Layer Decoupling in a Stripe-Ordered High-$T_c$ Superconductor, EDUARDO FRADKIN, UIUC, EREZ BERG, EUN-AH KIM, STEVE KIVELSON, Stanford University, VADIM OGANESEYAN, Yale University, JOHN TRANQUADA, Brookhaven National Laboratory, SHOUCHENG ZHANG, Stanford University — In the stripe-ordered state of a strongly correlated two-dimensional electronic system, under a set of special circumstances, the superconducting condensate, like the magnetic order, can occur at a nonzero wave vector corresponding to a spatial period double that of the charge order. In this case, the Josephson coupling between near neighbor planes, especially in a crystal with the special structure of $\text{La}_2\text{Ba}_2\text{Cu}_3\text{O}_6$, vanishes identically. We propose that this is the underlying cause of the dynamical decoupling of the layers recently observed in transport measurements at $x = 1/8$.


4:18PM W11.00010 Exact diagonalization study of electronic nematic and d-wave states, HYEONJIN DOH, THOMAS GRZESIAK, HAE-YOUNG KEE, University of Toronto — It was proposed that the d-density wave (ddw) and the electronic nematic states are relevant phases in the phase diagram of high $T_c$ cuprates. The two phases break different symmetries, and their order parameters have been used to describe the characteristic broken symmetries. Here we show that the two order parameters transform into each other under a local gauge transformation, which implies that the order parameters cannot represent different broken symmetric states, if a Hamiltonian is invariant under such a transformation. The two order parameters describe distinctly different states, when the nearest neighbor hopping integral is finite, but the states are nearly degenerate at a strong coupling limit. We also present a phase diagram of a Hamiltonian with correlated hopping, and nearest neighbor repulsive interactions using Lanczos exact diagonalization where we find an interesting interplay between the ddw and nematic states. We compare our results with the previous mean field calculation, and discuss a possible relevance to a d-wave superconducting state.

4:30PM W11.00011 Competition between superconductivity and antiferromagnetism as a boson-fermion mixture problem, GERARDO ORTIZ, LEONID ISAEV, Indiana University - Dep. of Physics, CRISTIAN D. BATISTA, Los Alamos National Laboratory — It is widely believed that the key to understanding the mechanism of superconductivity in cuprate materials and heavy fermion compounds lays in the competition between two quantum orders: superconductivity and antiferromagnetism, which complicates the choice of relevant effective degrees of freedom. Here we present a new isomorphic mapping, preserving the dimension of the on-site Hilbert space, where holons are represented by fermionic and spinons — by bosonic degrees of freedom, which, we claim, are the relevant ones in a certain regime (low density). Starting from t-J-like models we show that the original Hamiltonian can be exactly mapped onto a mixture of interacting fermion and boson gases. It is then demonstrated that this system may be considered as dilute under certain experimentally reasonable conditions. In this limit we show that the fermion gas exhibits a pairing instability, caused by a two boson exchange, which implies superconductivity of holons in the original repulsive model. Although the long-range Coulomb interaction is, in principle, capable of suppressing this state, we argue about a physical mechanism for its compensation, which is relevant for real materials. Our results also lead to a mechanism for superfluidity in ultracold boson — fermion gas mixtures.

4:42PM W11.00012 Stability of nodal quasi-particles in superconductors with coexisting orders, EREZ BERG, CHENG-CHIEN CHEN, STEVEN A. KIVELSON, Stanford University — The possible existence of nodal quasi-particles is one of the most distinctive properties of unconventional superconductors. Nodal quasi-particles have many unique experimental fingerprints, such as a linear temperature dependence of the superfluid density. It is therefore interesting to ask under what conditions can they exist generically. Here, we establish a condition for the perturbative stability of zero energy nodal points in the quasi-particle spectrum of superconductors in the presence of a general coexisting commensurate order. The nodes are found to be stable if the Hamiltonian commutes with the Fermi surface and is quasiperiodic under a specific lattice translation. The principle is demonstrated with a few examples. Some experimental implications of various types of assumed order are discussed in the context of the cuprate superconductors.

4:54PM W11.00013 S-wave superconductivity from predominantly d-wave pairing, PAUL ORETO, Department of Physics, Stanford University, BORIS SPIVAK, Department of Physics, University of Washington, Seattle, STEVEN KIVELSON, Department of Physics, Stanford University — We have studied the zero temperature properties of a system consisting of dilute superconducting droplets embedded in a weakly disordered Fermi liquid metal. Even under the assumption that the pairing interaction occurs exclusively in the d-wave channel, irregularities in the shape of the droplets, or impurities within the droplet generically induce local mixing of s-wave and d-wave components of the superconducting order. Moreover, we find that the Josephson coupling between the s-wave components of the order parameter on two droplets separated by a distance $r$ falls off as a slower power law than does the d-wave component. Thus, for dilute enough droplets, even if the local gap structure within each droplet is dominantly d-wave-like, the globally phase coherent portion of the superconducting order must have s-wave symmetry. We speculate that this effect could lead to a region of globally s-wave superconductivity in highly overdoped cuprates.

5:06PM W11.00014 Absence of superconductivity in the $\frac{1}{2}$-filled band Hubbard model on a triangular lattice, HONGTAO LI, University of Arizona, R. TORSTEN CLAY, Mississippi State University, S. MAZUMDAR, University of Arizona — The superconducting $\kappa$-(BEDT-TTF)$_2$X salts are strongly dimerized, with one hole per dimer unit cell. The occurrence of antiferromagnetism under ambient pressure, and the appearance of superconductivity under pressure has led several investigators to suggest that the superconductivity can be explained within an anisotropic triangular lattice $\frac{1}{2}$-filled band Hubbard Hamiltonian. Within this picture, pressure takes the system closer to the isotropic limit, when antiferromagnetism gives way to d-wave superconductivity. We have performed exact diagonalizations on a 16-site periodic anisotropic triangular lattice as a function of the Coulomb interaction (Hubbard U) and the anisotropy to investigate this claim. We calculate bond orders, double occupancies, spin-spin correlations, spin structure factors and $d_{\pi_x\sigma}$ Superconducting pair-pair correlations. We are able to confirm the Mott metal-insulator transition and antiferromagnetism, but we do not find any hint of long range superconducting correlations. Neither is there any region of the Hubbard U where these correlations are enhanced by the interaction strength.

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Thursday, March 13, 2008 2:30PM - 5:30PM – Session W12 DCMP: Metal Insulator Transition II: Theory Morial Convention Center 203

1 Supported by DE-FG02-06ER46315
2:30PM W12.00001 Effect of frustration on charge dynamics for a doped two-dimensional triangular Hubbard lattice. TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University — We examine the optical conductivity $\sigma(\omega)$ and the chemical potential $\mu$, together with the spin correlation, in the strong-coupling limit of a hole-doped two-dimensional triangular Hubbard model near half filling by using an exact diagonalization technique [1]. In contrast to the case of a square lattice without frustration, the doping dependences of $\mu$ and the Drude weight indicate that the charge degree of freedom is weakly coupled to the spin degree of freedom. However, we find that $\sigma(\omega)$ shows strong incoherent excitations extended to a higher energy region. This implies that geometrical frustration in strongly correlated electron systems influences incoherent charge dynamics. Momentum-dependent charge dynamics is also compared with that of the square lattice.

2:42PM W12.00002 Exact diagonalization analysis of the Anderson-Hubbard model and comparison to real-space self-consistent Hartree-Fock solutions. XI CHEN, Dept. of Physics, Queens University, PAKWON Leung, Dept. of Physics, Hong Kong University of Science and Technology, ROBERT GOODING, Dept. of Physics, Queens University — We have obtained the exact ground state wave functions of the Anderson-Hubbard model for different electron fillings on a 4x4 lattice with periodic boundary conditions. When compared to the uncorrelated ground states (Hubbard interaction set to zero) we have found evidence of very effective screening, producing smaller charge inhomogeneities due to the Hubbard interaction, particularly at 1/2 filling, and have successfully modelled these local charge densities with non-interacting electrons that experience a static screening of the impurity potentials. Further, we have compared such wave functions to self-consistent real-space unrestricted Hartree-Fock solutions and have found that these approximate ground state wave functions are very successful at reproducing the local charge densities, and may indicate the role of dipolar backflow in producing a novel metallic state in two dimensions.

2:54PM W12.00003 Electronic Griffiths phase near a disordered Mott transition in $D = 2$. ERIC ANDRADE, Florida State University and Univ. of Campinas, EDUARDO MIRANDA, Univ. of Campinas, VLAD DOBROSAVLJEVIC, Florida State University — We investigate the effects of weak and moderate disorder on the $T = 0$ Mott Metal-Insulator Transition (MIT) in two dimensions, by solving the disordered Hubbard Model within the so-called Statistical Dynamical Mean Field Theory (statDMFT) [1]. In the weak disorder regime, we recover the results of the standard DMFT limit [2], including strong disorder screened close to the MIT. For moderate disorder, the screening of the disorder remains strong, but is reduced by fluctuation effects absent in high dimensions. For disorder strength $W$ smaller then the on-site interaction $U$, the transition remains the Mott character, where the local quasiparticles weights $Z_i$ vanish on all sites at the transition, indicating the transmutation of all electron into local magnetic moments. In contrast to the behavior in high dimensions [2], the corresponding distribution function $P(Z)$ is found to assume a singular form as the transition is approached, indicating the emergence of an electronic Griffiths phase [3] preceding the MIT.

2:54PM W12.00004 An Exactly Solvable Model with a Tunable Mott Gap without Broken Symmetry. DANIEL HANSEN, B. SRIRAM SHAstry, UCSC Physics — The 1d Hubbard model at half filling provides the only known example of a Mott Hubbard insulating state, with a Mott charge gap without any concomitant broken symmetry. Such a state has inspired much current work in correlated matter in low dimensions. We present a model, where the Mott gap can be manipulated and in fact made to vanish with some parameter. Using the higher conserved currents found by Shastry in 1986 for the 1d Hubbard model, we construct a new model which does show a tunable Mott gap. The model is given by the hamiltonian

$$H = H_{\text{Hubbard}}(U) + \lambda I_3(U),$$

where $H_{\text{Hubbard}}$ is the Hubbard hamiltonian and $I_3$ is its third conserved current. The new model has exactly the same space time symmetries as the Hubbard model, but possesses two parameters, $U$, $\lambda$. The phase diagram in $\lambda - U$ is explored using numerical methods and the Bethe Ansatz. It displays several interesting features including a “superconducting" type state. A significant role is played by a band transition at $U = 0$ (similar to the Lifshitz transition), wherein the two fermi points of the Hubbard model break up into 6 Fermi points. We also find a variety of second order transitions.

3:30PM W12.00006 Insulator-Insulator Transitions in an Ionic Hubbard Model. ARA GO, GUN SANG JEON, Seoul National University — We study the ionic Hubbard model in one and two dimensions at zero temperature. As the Hubbard interaction is increased, the system is known to transform from a band insulator to a Mott insulator. The former phase is induced by the alternating on-site potential energy while the strong local Hubbard interaction drives the system towards correlated Mott insulator. In order to examine the transition nature, we perform the cellular dynamical mean-field calculation on a finite-size system, an exact diagonalization technique. From the computed local density of states we estimate the spectral gap as the interaction strength is varied. We also calculate the momentum-dependent density of states which exhibits characteristic features for different phases.

3:42PM W12.00007 The Anderson-Mott transition for a correlated 2D system. MARIA ELISABETTA PEZZOLI, FEDERICO BECCA, GIUSEPPE SANTORO, INFN-CNR Democritos and SISSA (Trieste), MICHELE FABRIZIO, INFN-CNR Democritos, SISSA, and ICTP (Trieste) — The interplay of disorder and electron-electron interaction can lead a bidimensional system to different phase transitions. We show that the Gutzwiller wave function generalized for an inhomogeneous system and with a long-term Jastrow factor provides a proper variational description of the Mott Hubbard insulating state, with a Mott charge gap without any concomittant broken symmetry. Such a state has inspired much current work in correlated systems. We construct a new model which does show a tunable Mott gap. The model is given by the hamiltonian

$$H = H_{\text{Hubbard}}(U) + \lambda I_3(U),$$

where $H_{\text{Hubbard}}$ is the Hubbard hamiltonian and $I_3$ is its third conserved current. The new model has exactly the same space time symmetries as the Hubbard model, but possesses two parameters, $U$, $\lambda$. The phase diagram in $\lambda - U$ is explored using numerical methods and the Bethe Ansatz. It displays several interesting features including a “superconducting" type state. A significant role is played by a band transition at $U = 0$ (similar to the Lifshitz transition), wherein the two fermi points of the Hubbard model break up into 6 Fermi points. We also find a variety of second order transitions.

3:54PM W12.00008 The 2D Metal-Insulator Transition: A percolative Monte Carlo study. DONALD PRIOUR JR., University of Missouri, Kansas City, SANKAR DAS SARMA, University of Maryland, College Park — We examine the metal-insulator transition (MIT) in two dimensional electronic systems (e.g. n doped GaAs heterostructures) in the presence of a long-range Coulombic random potential set up by a nearby layer of charged impurities. An iterative scheme taking into account nonlinear screening is used to obtain the inhomogeneous “landscape" of electron-rich and electron-depleted regions. The percolation (or not) of electron rich areas (in the regime of electronic densities $n$ where linear screening breaks down) is determined by a variant of the Hoshen Kopelman algorithm. Identifying the percolation transition as the metal-insulator transition, we calculate the critical electron density $n_c$ as a function of the concentration of charged impurities, the separation $d$ of the impurity layer from the electronic layer, and the thickness of the impurity rich region; the effect of correlated impurity positions is also examined. Using finite size scaling analysis, we calculate the critical exponent $\delta$ for the asymptotic scaling $\sigma \propto (n - n_c)^\delta$ in the vicinity of the MIT. We acknowledge support from US-ONR and NRI-NSF.
4:06PM W12.00009 Quantum and thermal fluctuation effects on solid-light systems . MARTIN HOHENADLER, University of Cambridge, MARKUS AICHHORN, University of Wuerzburg, CHARLES TAHAN, PETER LITTEWOOD, University of Cambridge — Several theoretical proposals of strongly correlated polariton systems which exhibit a quantum phase transition from a Mott insulator to a superfluid phase have recently been made. Here we study Mott phases of polaritons in a model of optical microcavities in a photonic crystal with nearest-neighbor photon hopping. The variational cluster approach takes into account quantum fluctuations exactly on the lengthscale of finite clusters, and yields phase diagrams and single-particle spectra at zero and finite temperature in one and two dimensions. The relation of the model to the well-known Bose-Hubbard model is explored, and implications of our findings concerning the stability of the Mott state at finite temperatures for technological applications are discussed.

4:18PM W12.00010 Effects of electron correlations on delocalization and percolation of electronic states . KENDALL MALLORY, Point Loma Nazarene University — A simulation of the effects of electron correlations on the formation of delocalized states and percolating clusters is presented. The model includes disorder in site locations and energy and uses a semi-classical approach to finding matrix elements and diagonalizing the Hamiltonian. We are also looking for scale invariant properties in the system.

4:30PM W12.00011 Dynamic mean-field theory of the ionic Hubbard model , JI-WOO LEE, Myongji University, Yong-In, South Korea, GUN SANG JEON, Seoul National University, Seoul, South Korea — We study the ionic Hubbard model in the infinite dimensions in the framework of dynamical mean-field theory. Exact diagonalization is used to obtain the impurity Green’s function to satisfy the self-consistent equation. We obtain a phase diagram in the parameter space of local ionic potential strength, $\Delta$ and local repulsive energy, $U$ exhibiting three phases: Mott insulator, metal, band insulator. Analyzing the spectral density, we compare our results with those of iterative perturbation theory and quantum Monte Carlo study in two dimensions.

4:42PM W12.00012 Evolution of the Mott-Hubbard insulator transition in bulk nonequilibrium; dynamical mean field theory . RYAN HEARY, JONG HAN, State University of New York at Buffalo — The equilibrium dynamical mean-field theory (DMFT) is extended to the steady-state nonequilibrium in which the Hubbard lattice is populated by left and right movers. The nonequilibrium boundary condition is imposed in the non-interacting limit by applying a chemical potential shift between the left and right movers of the homogeneous bulk system. The success of this theory lies in the fact that the local Green function can be calculated nonperturbatively using the imaginary-time formulation of the steady-state nonequilibrium [1]. We study the evolution of metallic quasi-particle excitations near the Mott-Hubbard insulator transition as a function of the chemical potential bias. The nonequilibrium DMFT algorithm will be presented along with the nonlinear nonequilibrium destruction of the Kondo resonance. [1] J. E. Han, R. J. Heary, Imaginary-time formulation of steady-state nonequilibrium: application to strongly correlated transport, accepted to Phys. Rev. Lett. arXiv:0704.3198.

4:54PM W12.00013 Non-local Coulomb correlations in metals close to a charge order insulator transition . JAIME MERINO, Universidad Autonoma de Madrid — Recent extensions of dynamical mean-field theory (DMFT) to clusters either in its real space (CDMFT) or momentum space versions (DCA) have become important tools for the description of electronic properties of low dimensional strongly correlated systems. In contrast to single site DMFT, short range correlation effects on electronic properties of systems close to the Mott transition can be analyzed. We have investigated the charge ordering transition induced by the nearest-neighbor Coulomb repulsion $V$ in the 1/4-filled extended Hubbard model using CDMFT. We find a transition to a strongly renormalized charge ordered Fermi liquid at $V_{CO}$ and a metal-to-insulator transition at $V_{MI}$. Short range antiferromagnetism occurs concomitantly with the CO transition. Approaching the charge ordered insulator, $V$<$V_{MI}$, the Fermi surface deforms and the scattering rate of electrons develops momentum dependence on the Fermi surface.

5:06PM W12.00014 Exact steady state non-equilibrium DOS of the Hubbard model . ALEXANDER JOURA, JIM FREERICKS, Georgetown University, USA; THOMAS PRUSCHKE, University of Goettingen, Germany — Using a non-equilibrium Kadanoff-Baym-Keldysh formalism, we derive exact equations relating the retarded Green’s function to the retarded self-energy for lattice electrons in presence of a constant and uniform electric field $E$. Such an approach allows us to go beyond linear response theory and study the behavior of systems for arbitrarily large electric fields. We find that the conventional dynamical mean-field theory (DMFT) algorithm is the same as in equilibrium except for a significantly modified lattice Dyson equation which couples together frequencies separated by the Bloch frequency. We apply the method to the Hubbard model and solve the model within the DMFT framework. As an impurity solver, we employ the numerical renormalization group (NRG). We discuss how the density of states (DOS) evolves as the electric field strength $E$ and interaction strength $U$ change. In particular, when both $E \ll 1$ and $U \ll 1$ the DOS is a set of equally spaced peaks (the so-called Wannier-Stark ladder). Increasing $U$ leads to a broadening of the peaks, which finally merge and then evolve into a DOS that is quite similar to the equilibrium DOS. Increasing $E$ while keeping $U \ll 1$ splits the peaks, resulting in novel behavior for the DOS, which is reminiscent of a metal-insulator transition (but the system carries current).

5:18PM W12.00015 Mott transition and Universality at finite temperatures . STEFANOS PAPANIKOLAOU, University of Illinois, Urbana-Champaign, RAFAEL M. FERNANDES, Instituto de Fisica “Gleb Wataghin”, Universidade Estadual de Campinas and Laboratorio Nacional de Luz Sincrotron, Campinas, SP, Brazil, EDUARDO FRADKIN, PHILIP W. PHILLIPS, University of Illinois, Urbana-Champaign, JOERG SCHMALIAN, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, RASTKO SKNEPNEK, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — We consider the finite temperature Mott critical point which has been the subject of recent experimental investigation. We demonstrate that this critical point is in the Ising universality class, consistent with all available experimental data. We show that, even though the thermodynamic behavior of the system near such a critical point is described by an Ising order parameter, the global conductivity depends on other singular observables and, in particular, the energy density, leading to the emergence of multiple crossover regimes. Finally, we show that in the presence of weak disorder the dimensionality of the system has crucial effects on the size of the critical region that is probed experimentally. ArXiv:0710.1627 and in press at Physical Review Letters.

**Thursday, March 13, 2008 2:30PM - 5:18PM – Session W13 DCOMP: Quantum Monte Carlo** Morial Convention Center 204
2:30PM W13.00001 The Continuous Time Quantum Monte Carlo method as a cluster solver in the Dynamical Cluster Approximation, KARLIS MIKELSONS, ALEXANDRU MACRIDIN, MARK JARRELL, University of Cincinnati, EMANUEL GULL, MATTHIAS TROYER, ETH Zuerich, Switzerland, SEBASTIAN FUCHS, THOMAS PRUSCHKE, University of Goettingen, Germany — We have investigated the application of the Continuous Time Quantum Monte Carlo (CTQMC) method, based on interaction expansion, to solve the Hubbard model within the Dynamical Cluster Approximation (DCA). We show that CTQMC reproduces results obtained with the well known Hirsch - Fye method (HFQMC), including non-perturbative phenomena. We discuss the advantages and limitations of CTQMC as a cluster solver in the DCA. Since any QMC method suffers from fermion sign problem at low temperatures and large system sizes, we present the results of a detailed study of the sign problem within CTQMC, and compare it to HFQMC. We also discuss potential extensions of (CTQMC+DCA) for treating the phases with broken symmetry.

2:42PM W13.00002 Continuous-time method for quantum impurity models, EMANUEL GULL, ETH Zurich, PHILIPP WERNER, Columbia University, OLIVIER PARCOLLET, Service de Physique Theorique, CEA/DSM/SPHT-CNRS/SPM/URA, MATTHIAS TROYER, ETH Zuerich — We present a new continuous-time quantum Monte Carlo algorithm for quantum impurity problems. The method allows an efficient simulation of large cluster impurity models with density density coupling. We compare the computational effort and average sign to alternative quantum Monte Carlo approaches, such as the discrete-time Hirsch-Fye algorithm [J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. 56, 2521 (1986)] and the weak coupling solver by Rubtsov, Savkin and Lichtenstein [Phys. Rev. B 72 035122 (2005)].

2:54PM W13.00003 Progress in the study of Molecular Hydrogen-Benzene binding†, TODD D. BEAUDET, MICHELE CASULA, JEONGNIM KIM, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — In this work we present a quantum Monte Carlo study of the hydrogen-benzene system where binding is very weak. We demonstrate that the binding is well described at both the VMC and DMC levels by a single determinant correlated geminal wave function1 with an optimized compact basis set that includes diffuse functions. Agreement between VMC and fixed node DMC binding energies is found to be within 0.16 mHa, suggesting the calculations are well-converged with respect to the basis. This relative insensitivity to basis set and superposition error is an advantage of the QMC methods we employ. Comparison is made with a Slater-Jastrow wave function at the DMC level using a trial function comprised of PBE single-body orbitals, empirical models and previous work2. The physical underpinnings of the interaction will be discussed including the role of diffuse basis functions in this system. Progress on systems where binding is expected to be more favorable for practical hydrogen storage will also be presented.

† Supported by NSF DMR03-75393 and A0602 ArmyUMC00050713

3:06PM W13.00004 Geometry optimization with a noisy potential energy surface, JEFFREY GROSS-MAN, LUCAS WAGNER, University of California, Berkeley — Molecular and solid systems in the excited state and in the weak-binding regime (for example) are often not described well by current density functional(DFT) methods, often leading to inaccurate minimum energy structures. Quantum Monte Carlo(QMC) is a tempting method to improve on these deficiencies, since it offers a highly accurate fully correlated first principles description. However, QMC suffers from two major deficiencies: 1) forces are not easily calculated and 2) the energy is obtained with stochastic uncertainty, which makes optimization a challenging task. We examine several ways of compensating for this uncertainty while only using the reliable total energies obtained in QMC.

3:18PM W13.00005 Quantum Monte Carlo calculations of NiO, RYO MAEZONO, Japan Advanced Institute of Science and Technology, Japan., MIKE D. TOWLER, RICHARD. J. NEEDS, TCM, Cavendish Laboratory, University of Cambridge, U.K. — We describe variational and diffusion quantum Monte Carlo (VMC and DMC) calculations [1] of NiO using a 1024-electron simulation cell. We have used a smooth, norm-conserving, Dirac-Fock pseudopotential [2] in our work. Our trial wave functions were of Slater-Jastrow form, containing orbitals generated in Gaussian-basis LHY periodic calculations. Jastrow factor is optimized using variance minimization with optimized cutoff lengths using the same scheme as our previous work. [4] We apply the lattice regulated scheme [5] to evaluate non-local pseudopotentials in DMC and find the scheme improves the smoothness of the energy-volume curve.


3:30PM W13.00006 Efficient orbital storage and evaluation for quantum Monte Carlo simulations of solids, KENNETH ESSLER, Carnegie Institution of Washington — Researchers have applied continuum quantum Monte Carlo methods to solids with great success, but thus far applications have been largely limited to crystals with simple geometry. In these simulations, three-dimensional cubic B-splines have proven to be a fast and accurate means of storing and evaluating electron orbitals. While B-splines require less memory than other spline interpolation schemes, modern cluster nodes often have insufficient memory to store the orbitals for more complex systems. We introduce three techniques, appropriate in different circumstances, to dramatically reduce the memory required for orbital storage, while retaining high accuracy: the generalized tiling of primitive-cell orbitals into a supercell of arbitrary shape, the use of nonuniform grids for localized orbitals, and the periodic replication of localized orbitals. We give examples for cubic boron nitride and wüstite (FeO), and show that these methods can reduce the memory used for orbital storage by more than two orders of magnitude. Finally, we introduce an open-source B-spline library to facilitate the incorporation of these methods into QMC simulation codes.

3:42PM W13.00007 Triplet pairings and fermion wave functions nodal topologies, LUBOS MITAS, MICHAL BAJDICH, SHUMING HU, North Carolina State University — Fixed-node quantum Monte Carlo methods rely on accurate fermion nodes of trial wave functions. Recently, we have shown that BCS wave functions possess for generic singlet ground states possess the correct minimal number of two nodal cells. This contrasts with the Hartree-Fock wave functions which exhibit higher counts of four or more nodal domains resulting in incorrect nodal topologies. We prove that for fully spin-polarized systems one can show the same effect. As a simple example, we consider the HF wave function for the lowest quartet of S symmetry and even parity for three electrons in a Coulomb potential. The wave function of this state $1S(1s2s\bar{3}s)$ has six nodal cells corresponding to $3!$ reordering of the radii. We show that paffian with triplet pairings is the simplest wave function which has the correct topology with two nodal cells. We further expand the study to some exactly solvable models to study the exact nodal structures dependence on potentials.
3:54PM W13.00008 Compact and accurate quantum Monte Carlo wave functions for first-row atoms\textsuperscript{1}. F. R. PETRZIELO, LASSP, Cornell University, JULIEN TOULOUSE, Universite Pierre et Marie Curie, Paris, France, W. A. AL-SAIDI, C. J. UMRIGAR, LASSP, Cornell University, R. G. HENNIG, Materials Science and Engineering, Cornell University — Many-body wave functions for the first row atoms (Li to Ne) are represented as expansions in eigenstates of $L^2, L_z, S^2, S_z$ multiplied by a Jastrow factor. This configuration state function (CSF) expansion provides a systematic means for improving a wave function by including CSFs corresponding to higher excitations. Optimization of all wave function parameters including Jastrow, CSF and orbital coefficients as well as basis exponents, starting from a simple initial guess, results in compact and accurate wave functions (low energy and variance of local energy). Further improvements by use of backflow transformations are explored. This work aims to develop insight into selecting the relevant CSFs particularly for large systems, where it is difficult to include all CSFs to a given order.

\textsuperscript{1}Supported by an NDSEG fellowship and by NSF and DOE

4:06PM W13.00009 A DQMC study of cohesion energy of small Li clusters based on an RVB nodal structure\textsuperscript{1}. DANIEL NISSENBAUM, Northeastern University, LEONARDO SPANU, UC Davis and SISSA, Italy, CLAUDIO ATTACALITE, SISSA, Italy, BERNARDO BARBIELLINI, ARUN BANSIL, Northeastern University — We have carried out a diffusion Quantum Monte Carlo study (DQMC) of the cohesion energy of small (2, 4, and 8 atom) Li clusters based on Resonating Valence Bond (RVB) wavefunctions, and compared the results to the corresponding values obtained via wavefunctions utilizing a typical Hartree-Fock (HF) nodal structure (Jastrow-Slater wavefunctions). The RVB wavefunction allows more flexibility in the nodal structure than the HF wavefunction, and yields some improvement in the cohesion energy of Li$_2$, with comparable gain for the larger clusters. Interestingly, the variance of the local energy for the variationally optimized (VQMC) RVB wavefunction is found to be significantly smaller than for the VQMC-optimized Jastrow-Slater wavefunction, resulting in faster convergence of the DQMC calculations. This would make the RVB wavefunction a promising candidate for investigating larger and more complicated clusters.

\textsuperscript{1}Work supported in part by the USDOE

4:18PM W13.00010 An Improved Pressure Estimator for quantum Monte Carlo\textsuperscript{1}. JEREMY MCMINIS, JEONGNIM KIM, DAVID CEPERLEY, Department of Physics, University of Illinois, CARLO PIERLEONI, Department of Physics, University of L’Aquila — Assaraf and Caffarel have developed a systematic method for deriving reduced variance estimators for observables for quantum Monte Carlo calculations and have applied to forces[1], the one body density and the spherical and system averaged pair density. It has yet to be applied to a thermodynamic observable. In this work we derive an expression for an improved pressure estimator for use in variational Monte Carlo and diffusion Monte Carlo calculations. We show that because the dependence of the trial wave function on the density is known, for the homogeneous electron gas this new estimator is accurate and efficient to implement. We discuss its application to many-body Hydrogen at high pressure. [1] Roland Assaraf and Michel Caffarel, J. Chem. Phys. 113, 4028 (2000)

\textsuperscript{1}The work performed at the Materials Computation Center was supported by the National Science Foundation under grant no. DMR-03 25939 ITR, and through the Frederick Seitz Materials Research Laboratory (U.S. Dept. of Energy grant no. DEFG02-91ER45439).

4:30PM W13.00011 The Model Periodic Coulomb interaction in k-space: modelling the spherically averaged structure factor. RENE GAUDOIN. Donostia International Physics Center (DIPC), Manuel de Lardizabal Pasealeku, E-20018 Donostia, Basque Country, Spain, IDOIA GURTUBAY, Materia Kondentsatuaren Fisika Saila, Zientzia eta Teknologia Fakultatea, Euskal Herririo Unibertsitatea, PO 644, E-48080 Bilbo, Basque Country, Spain, TXEMA PITARKE, CIIC nanGUNE Consolider, Mikeltegi Pasealeku 56, E-2009 Donostia, Basque Country, Spain — Within Quantum Monte Carlo (QMC) calculations the Model Periodic Coulomb (MPC) interaction is a well known method to reduce finite size effects related to the long range nature of the Coulomb interaction. Recently we presented a method based on modelling the continuous-k spherically averaged structure factor (SF) to understand and reduce Coulomb finite size effects. Here we show that our SF based method can be viewed as k-resolved MPC. This allows us to analyse the implicit assumptions that underlie MPC and what to do when these assumptions are not justified, i.e. in non-interaction Hartree-Fock systems or even surfaces. While we present data for the homogeneous electron gas the method itself is general.

4:42PM W13.00012 Backflow transformation improves QMC calculations of silicon self-interstitial defects\textsuperscript{1}. WILLIAM D. PARKER, KEVIN P. DRIVER, JOHN W. WILKINS, Ohio State University, RICHARD G. HENNIG, Cornell University — Recent advances in quantum Monte Carlo (QMC) reduce error introduced by approximations. Direct improvement of the trial wave function through backflow transformation of the electron coordinates\textsuperscript{1} produces a wave function closer to the ground state by moving electrons out of the way of a given electron. Adding plane waves of particle position to the Jastrow factor\textsuperscript{2} augments the accounting for interparticle correlation in QMC calculations by capturing the “corners” of the simulation cell neglected when the Jastrow is only a function of pair separation. Hybrid density functionals have produced better starting trial wave functions for molecules by incorporating some exact exchange to more accurately describe electron-electron interactions. We apply backflow transformation, plane-wave-expanded Jastrow factors and hybrid functional trial wave functions to QMC calculations of silicon self-interstitial defects. [1] Lopez-Rios et al., Phys. Rev. E 74, 066701 (2006). [2] Drummond et al., Phys. Rev. B 70, 235119 (2004).

\textsuperscript{1}Support from DOE (DE-FG02-99ER45795) and computing resources from Ohio Supercomputing Center and NERSC.

4:54PM W13.00013 Density Dependence of Fixed-Node Errors. KEVIN RASCH, LUBOS MITAS, Center for High Performance Simulation, Dept of Physics, North Carolina State University — With both variational and diffusion Monte Carlo (VMC and DMC) methods, we calculate the ground state energy of isoelectronic free ions in the first row of the periodic table for both Hartree-Fock and Configuration Interaction based trial wave functions. As it is well-known, the fixed-node DMC is exact in the limit that the fermion nodes of the trial wave function are also exact. This study is focused on understanding the density dependence of the fixed-node error since one expects that with increasing density of electrons the errors would be more pronounced due to higher frequency of sampling of the nodal regions and/or areas with low potential energy. For this purpose we construct Hartree-Fock and multi-reference wave functions and quantify the fixed-node biases. We compare strongly bonded highly localized cations, neutral atoms and weakly bonded anions. We compare the absolute and relative sizes of fixed-node errors and their relationships to multi-reference wave functions.

5:06PM W13.00014 Slater determinant and pfaffian expansions for wave functions in electronic structure quantum Monte Carlo. MICHAL BAJDICH, LUBOS MITAS, CHIPS, Department of Physics, North Carolina State University — We investigate several types of expansions in Slater determinants and pfaffians for trial wave functions in fixed-node quantum Monte Carlo. The long expansions in determinants are analyzed in order to identify the terms with the largest contributions towards decreasing the fixed-node errors. We further investigate the efficient mapping of these terms onto pfaffian expansions. We apply this technique to test the cases of molecular and atomic systems and we discuss the amounts of recovered correlation energy relative to the expansion size. Finally, following upon our previous study [1], we explore how multiple Slater determinants and pfaffians for the accurate description of the wave functions of simple solids. [1] M. Bajdich et al. Phys. Rev. Lett. 96, 130201 (2006).
Quantum analysis of nonlinear beam splitter with second order nonlinearity.

W-system fields leads to the formation of a new type of EIT system: a Bose-Einstein condensate (BEC) trapped in a double well potential. A weak probe propagates through one of the wells and interacts with atoms in a three-level coherent superposition of its center–of–mass motion, if the wavelength is comparable to the well separation and if the external state of the atom is post-selected.

Simultaneously used for slowing down and generating higher vibrational states, but beyond the Lamb-Dicke regime concerning the tunneling split groundstate. The first case leads to an extended Jaynes-Cummings model which can be solved exactly. We show that the coupling between internal and external degrees of freedom of the atom induced by the cavity mode can provide a coherent coupling between identical electronic states in the two wells that leads to the formation of inter-well dressed states.

The inter-well coupling results in the formation of two ultra-narrow absorption resonances for the probe field that are inside of the ordinary EIT transparency window, which can be interpreted in terms of the inter-well dressed states and the formation of a novel type of dark state involving the coupling laser and the inter-well tunneling. To either side of these ultra-narrow resonances there is normal dispersion with ultra-large slope controlled by $g$. For realistic values of $g$, the large slope of this dispersion yields group velocities for the probe field that are two orders of magnitude slower than standard EIT systems. Additionally, we discuss the effects of the inter-well coupling on the nonlinear susceptibility, $\chi^{(3)}$.

Electromagnetically-induced transparency (EIT) in a four-level atom system

By turning off one of the two probe fields, a standard EIT behavior can be recognized in two independent V-systems. Our novel EIT technique is applied to ultra-cold Mg atoms in low-lying states. The density matrix formalism is employed for finding coherences between Zeeman levels of the upper $\text{^1P}_1$ state in our W-system. Solving the master equation for a population-trapped four-level atom system and assuming a zero population density on the Zeeman levels of the $\text{^1P}_1$ state give atomic susceptibilities for the dark states associated to the two probe fields. The analysis of the EIT behavior in our W-system is done by varying (1) the Rabi frequencies for the triplet state and (2) the detuning of the two probe lasers. The dependence of the EIT features with the B-field is also discussed.

Coherent optical spectroscopy of a strongly coupled semiconductor microcavity quantum-dot system

We describe recent experiments in which a fiber taper waveguide is used to perform steady-state coherent linear and nonlinear optical spectroscopy of a strongly coupled microcavity–QD system, probing the system on its photonic channel (rather than its matter channel, as in PL). Under weak driving, vacuum Rabi splitting is observed, while increasing the drive strength reveals saturation for an average intracavity photon number of less than one. (1) K. Srinivasan and O. Painter (2007), to appear in Nature, Dec. 6, 2007 (preprint: physics/0707.3311).

Monitoring electron spin decoherence in a quantum dot by weak measurement

This work was supported by Hong Kong RGC Project 2160322

Spontaneous emission from a tunneling atom

We study the tunneling of a two-level atom in a double well potential in which the atom couples either to a single electromagnetic field mode of a cavity to the full continuum of electromagnetic modes in three dimensions. Both studies are within the Lamb-Dicke regime concerning transitions to higher vibrational states, but beyond the Lamb-Dicke regime concerning the tunneling split groundstate. The first case leads to an extended Jaynes-Cummings model which can be solved exactly. We show that the coupling between internal and external degrees of freedom of the atom induced by the cavity mode can dramatically change the tunneling behavior. In general the tunneling process becomes quasiperiodic. If the cavity is fed with a coherent state, a collapse and revival of the tunneling can occur. Accessing the internal degrees of freedom of the atom with a laser allows to coherently manipulate the atom position, and in particular to prepare the atom in one of the two wells. In the second case, the tunneling process may decohere, depending on the wavelength corresponding to the internal transition and on the spontaneous emission rate. Interference fringes appear in the emitted light from a tunneling atom, or an atom in a stationary coherent superposition of its center–of–mass motion, if the wavelength is compatible to the well separation and if the external state of the atom is post-selected.

Session W14 DAMOP: Quantum Optics Morial Convention Center 205
3:42PM W14.00007 Single photon nonlinearities using arrays of cold polar molecules, T. BRAGDON, R. M. RAJAPAKSE, University of Connecticut, A. M. REY, ITAMP, S. F. YELIN, University of Connecticut, ITAMP — We model single photon nonlinearity via dipole-dipole interaction in cold polar molecules using the protected Dicke-like symmetric manifold for potential optical quantum computation processing. We report on potential decoherences described by phonon dispersion, spontaneous, and stimulated decays. We compare to individually addressed molecules from previous work, and discuss briefly the feasibility in optical quantum computation processing as an element of a controlled-Z gate.

3:54PM W14.00008 Fermionization of strongly interacting photons in one-dimensional nonlinear medium, DARRICK CHANG, VLADIMIR GRITSEV, Harvard University, GIOVANNA MORIGI, University of Barcelona, VLADAN VULETIC, MIT, MIKHAIL LUKIN, EUGENE DEMLER, Harvard University — Understanding strongly correlated quantum systems is a central problem in many areas of physics. The collective behavior of interacting particles gives rise to a variety of phenomena such as condensation in quantum chromodynamics, spontaneous symmetry breaking and phase transitions, and electron fractionalization in one dimensional systems and in the quantum Hall regime. While such systems typically involve strongly interacting massive particles, optical photons can also interact with each other in a nonlinear medium. In practice, however, such interactions are typically very weak. We describe a novel technique that allows the creation of a strongly correlated quantum gas of photons, which is made possible by the tight field confinement that can be achieved in a number of novel, one-dimensional optical systems. This confinement enables the generation of large optical nonlinearities via the interaction of photons with a nearby cold atomic gas, which can be further amplified by an optical Bragg grating that traps these photons within the medium. In its extreme, we show that a quantum light field can undergo fermionization in such one-dimensional media, which can be probed via standard photon correlation measurements. Realization of such systems can open a route for quantum simulators of matter Hamiltonians using light fields and novel applications in metrology and quantum information.

4:06PM W14.00009 Entangled-photon absorption in semiconductor nanostructures, FELIPE VALLEJO, LUIS QUIROGA, Universidad de los Andes — We present a comparative study of two-photon absorption by semiconductor nanostructures for two kind of light: (i) Light with wave-like classical properties (laser light) and (ii) A new type of quantum entangled light. First, we report on results concerning entangled-photon absorption processes due to a novel class of collisional processes in coreshell quantum dots. Second, we use the framework of the effective-mass approximation both the classical as well as the entangled two-photon absorption in quantum wells (QWs) and quantum wires (QWRs) have been addressed. Results for non-entangled light with polarization both parallel and perpendicular to the directions of confinement are in perfect agreement with the ones already known. We proceed to extend those results to the less explored case of entangled light absorption in semiconductor nanostructures. The absorption spectra for entangled light is richer in structure and complexity as compared with the classical light class. We find that the absorption rate (cross-section) for entangled light depends additionally on a new important parameter, the entanglement time $T_e$, which gives rise to quantum interference effects. As a result, entangled photons produce entangled-induced transparencies.

4:18PM W14.00010 Photon Tunneling Through Dielectric Bandgaps and Evanescent Gaps, NATALIA RUTTER, SERGEY POLYAKOV, PAUL LETT, ALAN MIGDALL, NIST, Gaithersburg, MD — We implement an optical tunneling testbed using the precise simultaneity of creation of twin photons produced by parametric down conversion and a Hong-Ou-Mandel interferometer. With this setup, we can measure photon traversal times of a sample with fs precision. We use this setup to compare the time for a photon to traverse dielectric stacks of odd versus even numbers of layers of alternating indexes of refraction. Preliminary data shows that subtle changes in the stack structure result in dramatic variations in photon traversal times ($\sim 10$ fs) that can range from sub- to super-luminal. Our ultimate goal is to use this setup to investigate photon tunneling times in regions of true evanescent propagation and compare them to the traversal times in our dielectric stack bandgap samples where the propagation is oscillatory. This allows us to test the suitability of certain optical models of tunneling and highlight the pitfalls that occur when relying on conditional measurements.

4:30PM W14.00011 Nonlinear wave scattering by small barrier potentials, WENJIE WAN, JASON W. FLEISCHER, Princeton University — Scattering by a barrier potential is a fundamental problem in wave physics, involving issues of boundary conditions, resonances, radiation, etc. While scattering in the linear case is well-known, the nonlinear case has received far less attention. In the nonlinear regime, self-interaction affects tunneling and re-radiation dynamics, often leading to new topological structures (e.g. dark solitons and vortices). Examples include molecules of both quantum and classical systems, plasmons, and nonlinear optics. Here, we focus on the optical case by considering plane-wave scattering from an optically-induced barrier potential (step index) inside a photorefractive crystal. We experimentally demonstrate shock wave formation (dark soliton trains) in 1D and vortex generation in 2D, as a function of barrier height and input wave angle. We show numerically that these results arise from a combination of tunneling, scattering, and Optical superflow around the boundary. Applications both within and beyond optics will be discussed.

4:42PM W14.00012 Photon localization and Dicke superradiance in atomic gases: crossover to a “small world” network, ERIC AKKERMANS, Technion and Yale University, AHARON GEROS, Technion, ROBIN KAISER, Nice University — We study photon propagation in a gas of $N$ atoms, using an effective Hamiltonian that accounts for photon mediated atomic dipolar interactions. The configuration average density $P(\Gamma)$ of photon escape rates is obtained from the spectrum of the $N \times N$ random matrix $\Gamma_{ij} = \sin(x_{ij})/x_{ij}$, where $x_{ij}$ is the dimensionless random distance between the $i$th and $j$th atoms. A scaling function is defined to study photons escape rates as a function of disorder and system size. We show that for a strong enough disorder, photons do not escape the gas. This localization is described using a mapping of this problem onto statistical properties of random networks. We show that there is no localization phase transition as expected in disordered systems typically involving strongly interacting massive particles, optical photons can also interact with each other in a nonlinear medium. In practice, however, such interactions are typically very weak. We describe a novel technique that allows the creation of a strongly correlated quantum gas of photons, which is made possible by the tight field confinement that can be achieved in a number of novel, one-dimensional optical systems. This confinement enables the generation of large optical nonlinearities via the interaction of photons with a nearby cold atomic gas, which can be further amplified by an optical Bragg grating that traps these photons within the medium. In its extreme, we show that a quantum light field can undergo fermionization in such one-dimensional media, which can be probed via standard photon correlation measurements. Realization of such systems can open a route for quantum simulators of matter Hamiltonians using light fields and novel applications in metrology and quantum information.

4:54PM W14.00013 Fermi two atom problem in extended Fredrichs-Lee Model, KAVAN MODI, JAMES ZABEL, GEORGE SUDARSHAN, The University of Texas at Austin — In 1932 Fermi calculated the time required for excitation transition between two atoms. He found the minimum time to be the distance between the atoms divided by the speed of light. Recently, Hegerfeldt, using a very basic argument of analyticity of the wavefunction, showed that the excitation amplitude of the second atom must be finite for all times or zero for all times. We are studying this problem in detail using a modified Fredrichs-Lee model where two discrete states are connected by a continuum. We can solve for the transition amplitude exactly in our model, without assuming that a photon is the mediator between the two discrete modes. Our model should shed some light on the conceptual difficulties that have bothered the community for long.

Thursday, March 13, 2008 2:30PM - 5:18PM — Session W15 GQI: Quantum Entanglement II, Morial Convention Center 207
2:30PM W15.00001 Experimental demonstration of anyonic statistics with multichain entanglement.  
HARALD WEINFURTER, WITLEF WIECZOREK, CHRISTIAN SCHMID, NIKOLAI KIESEL, REINHOLD Pohlner,  
University of Munich, Max-Planck-Institute for Quantum Optics, Germany, JIANNIS PACHOS, University of Leeds, UK — Particles in nature are usually distinguished  
according to their statistics in two categories: bosons and fermions. However, if one considers only two spatial dimensions statistical behaviour ranging from  
bosonic to fermionic is found. Particles exhibiting such a behaviour are called anyons. Our experimental demonstration of anyonic statistics is based on a  
particular two-dimensional model: the toric code proposed by Kitaev [1]. There, anyons arise as excitations that are generated by local operations. We show  
that for this model anyonic behaviour is revealed for as little as four qubits [2]. This enabled us to experimentally demonstrate anyonic statistics in a quantum  
simulation with four-phonon entanglement.


2:42PM W15.00002 Entanglement entropy and other observables of topological phases with  
finite correlation length. STEFANOS PAPANIKOLAOU, University of Illinois, Urbana-Champaign, KUMAR S. RAMAN, University of California,  
Riverside, EDUARDO FRADKIN, University of Illinois, Urbana-Champaign — We elucidate the topological features of the entanglement entropy of a region in  
two dimensional quantum systems with a finite correlation length. Firstly, we suggest that simpler reduced quantities, related to the von Neumann entropy, could be  
deﬁned to compute the topological entropy. We use our methods to compute the entanglement entropy for the ground state wave function of a quantum  
eight-vertex model in its topological phase, and show that a finite correlation length adds corrections of the same order as the topological entropy which come  
from sharp features of the boundary of the region under study. We also calculate the topological entropy for the ground state of the quantum dimer model on a  
triangular lattice by using a mapping to a loop model. The topological entropy of the state is determined by loop conﬁgurations with a non-trivial winding  
umber around the region under study. Finally, we consider extensions of the Kitaev wave function, which incorporate the effects of electric and magnetic charge  
ﬂuctuations, and use it to investigate the stability of the topological phase by calculating the topological entropy. arXiv: 0709.0729

2:54PM W15.00003 Valence-Bond Monte Carlo for Chains of Non-Abelian Quasiparticles. HUAN  
TRAN, NICK BONESTEEL, Department of Physics and NHMFL, Florida State University — In non-Abelian FQH states, quasiparticles carry quantum numbers  
(topological charge) which characterize a degenerate Hilbert space. When these quasiparticles are close enough together, the degeneracy of this Hilbert space is  
lifted and the quasiparticles are said to interact. Here we show that the valence-bond Monte Carlo method introduced by Sandvik for spin-1/2 systems can be  
generalized to simulate 1D chains of such interacting non-Abelian quasiparticles. For uniform chains, our Monte Carlo results for the ground state energy agree  
with known exact values. For random chains we conﬁrm numerically that, as expected, the ground state freezes into a random singlet phase. By suitably  
generalizing the notion of valence-bond entanglement entropy to the non-Abelian case we also conﬁrm the predicted result that in this phase the entropy of a  
block of length L scales as $S_L \sim \frac{d}{\ln L}$, where $d$ is the quantum dimension of the quasiparticles. Work supported by US DOE.

1A. Feiguin et al., PRL 98, 160409 (2007).

3:06PM W15.00004 Geometry of metal-insulator transitions in one-dimension. NOAH BRAY-ALI,  
University of Southern California, LORENZO CAMPOS VENUTI, Quantum Information Group, Institute for Scientific Interchange (ISI), Viale Settimio Severo  
65, I-10133 Torino, Italy, MARCO COZZINI, Dipartimento di Fisica, Politecnico di Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy, Quantum  
Information Group, Institute for Scientific, PAOLO ZANARDI, Quantum Information Group, Institute for Scientific Interchange (ISI), Viale Settimio Severo 65,  
I-10133 Torino, Italy, Univ. of Southern Califor. — We use the geometric approach to quantum critical points to study the metal-insulator transitions driven by  
chemical potential, or repulsion, $U$, in the one-dimensional Hubbard model. The transition to the band-insulator, as $U \rightarrow U_c$, exhibits conventional scaling  
of the ground-state fidelity metric tensor $G_{\mu,\nu} \equiv \text{Re} \left[ \langle \partial_\mu \psi \partial_\nu \psi \rangle - \langle \partial_\mu \psi \rangle \langle \partial_\nu \psi \rangle \right]$. For example, the metric diverges as $G_{U/V} \sim 1/n$, where, $n \sim \sqrt{U-U_c}$,  
is the band filling. At the Mott transition, the metric behavior depends on the path of approach to the critical point.

3:18PM W15.00005 Topological order at finite temperature: protected or not protected?  
CLAUDIO CASTELNOVO, University of Oxford, CLAUDIO CHAMON, Boston University — We investigate the behavior of the entanglement and topological  
order in the two- and three-dimensional toric code at finite temperature. From our results, we infer that quantum topological order is fragile with respect to  
thermal fluctuations in spite of the presence of a finite energy gap at zero temperature. In two dimensions, all topological order evaporates at any non-vanishing  
temperature in the thermodynamic limit. On the contrary, in three dimensions not all topological information is lost, although the topologically protected  
quantum information (qubit) stored in the ground state of the system is immediately degraded to topologically protected classical probabilistic information (pbit)  
at any infinitesimal temperature, in the thermodynamic limit. All information is eventually lost beyond a finite temperature phase transition. We comment on  
the implications of our results with respect to braiding operations and topological quantum computing.

3:30PM W15.00006 Long distance entanglement mediated by gapped spin chains. AIORES FERREIRA,  
JOAO LOPES DOS SANTOS, CFP and Dept Fisica, Faculdade de Ciencias da Universidade do Porto — This talk will describe an analytical approach for the  
computation of Long Distance Entanglement (LDE) mediated through one-dimensional quantum spin chains recently found in numerical studies [1]. I review  
the formalism that allows the computation of LDE for weakly interacting probes with gapped many-body systems and show that, at zero temperature, a DC  
response function determines the ability of the physical system to develop genuine quantum correlations between the probes. In the second part of the talk, I  
show that the biquadratic Heisenberg spin-1 chain is able to produce LDE in the thermodynamical limit and that the finite antiferromagnetic Heisenberg chain  
maximally entangles two spin-1/2 probes very far apart. This is of crucial importance since feasible mechanisms of entanglement extraction from real solid state  
systems and their ability to transfer entanglement between distant parties are essential ingredients for the implementation of Quantum Information protocols,  
such as teleportation or superdense coding.

3:42PM W15.00007 Entanglement of Impurities in Spin Chains1, ERIK SORENSEN, McMaster, NICOLAS LAFORENCIE, UP-sud, MING-SHYANG CHANG, IAN AFFLECK, UBC — Entanglement in $J_1 - J_2$, $S = 1/2$ quantum spin chains with an impurity is studied using analytic methods as well as large scale numerical density matrix renormalization group methods. The impurity contribution to the uniform part of the entanglement entropy, $S_{imp}$, is defined and analyzed in detail both in the gapless, $J_2 \leq J_1$, as well as the dimerized phase, $J_2 > J_1$, of the model. This quantum impurity model is in the universality class of the single channel Kondo model and we show that in a quite universal way the presence of the impurity in the gapless phase, $J_2 \leq J_1$, gives rise to a large length scale, $\xi_K$, associated with the screening of the impurity, the size of the Kondo screening cloud. The universality of the Kondo screening imprints scale of the form $S_{imp}(L)/S_{Kondo}(L)$ for a system of size $L$. At the critical point, $J_2^c$, an analytic approach based on a Fermi liquid picture, valid at distances $r \gg \xi_K$ and energy scales $T < T_K$, is developed and analytic results at $T = 0$ and $T \neq 0$ are obtained. In the dimerized phase an appealing picture of the entanglement is developed in terms of a thin soliton (TS) ansatz permitting variational calculations and the notions of impurity valence bonds (IVB) and single particle entanglement (SPE) are introduced.

1We acknowledge support from NSERC, CIAR, CFI and SHARCNET.

3:54PM W15.00008 Entanglement Entropy of States with Long-Range Magnetic Order, WENXIN DING, NICHOLAS BONESTEEL, KUN YANG, FSU & NHMFL — We study the bipartite entanglement entropy of spin models whose ground states have perfect ferromagnetic (FM) or antiferromagnetic (AFM) long-range order. For the FM case the entanglement entropy is taken to be one-half the quantum mutual information so as to properly take into account the ground state degeneracy. The calculation of the entropy for this case is then straightforward and agrees with previous work using a different approach. For the AFM case the problem is reduced to that of four coupled spins. This simplification allows us to determine the asymptotic behavior of the entropy analytically with results which agree well with exact numerical calculations. In both the FM and AFM cases we find the entropy grows logarithmically with block size, $N_1$. For example, if we take $N_1 = N/2$, where $N$ is the total number of spins, then in the FM case the entropy, $E$, scales as $E \approx \frac{1}{2} \ln N_1$, and in the AFM case, $E \approx \ln N_1$. In both cases the area law is clearly violated. Implications of these results for more general states with long range order are also discussed.

4:06PM W15.00009 Entanglement Entropy in the Two-Dimensional Random Transverse Field Ising Model1, STEPHAN HAAS, Department of Physics and Astronomy, University of Southern California, RONG YU, Department of Physics and Astronomy, University of Southern California and Department of Physics, University of Tennessee, HUBERT SALEUR, Service de Physique Theorique, CEN Saclay, Gif Sur Yvette, F-91191, France — We have applied the numerical strong disordered renormalization group method to the two-dimensional random transverse field Ising model, and studied the scaling behavior of the entanglement entropy. The leading term of the entanglement entropy scales linearly with the block size, following the so-called area law. However, besides this area law contribution, a subleading logarithmic correction at the quantum critical point is resolved. This correction is understood from the point of view of an underlying percolation transition, both at finite and at zero temperature.

1This work was supported by DOE, Grant No. DE-FG02-05ER46240. Computational facilities have been generously provided by the HPCC-USC Center.

4:18PM W15.00010 Entanglement Entropy and Complexity in Random Systems1, RODRIGUEZ-LAGUINA JAVIER, Mathematics Dept, Universidad Carlos III, Madrid (Spain) — Entanglement is considered to be the hallmark of quantum physics, and entanglement entropy (EE) is one of its most natural measurements. Its utility as a marker for quantum criticality for random systems is well established. Recently, it has been shown that the scaling of the running-time in some quantum annealing methods is also related to it. In this work we show how the behaviour of this magnitude in some random systems can provide insight about the complexity of the structure of their quantum critical points. Moreover, we provide some hints that point towards a relation between the behaviour of the EE and the complexity class of classical problems. References: J. Rodriguez-Laguna, J. Phys. A: Math. Theor. 40, 12043 (2007), and JSTAT P05008 (2007).

1Work supported by Spanish MEC, project FIS2006-04885.

4:30PM W15.00011 Entanglement Entropy Scaling in the Disordered Golden Chain, LUKASZ FIDKOWSKI, GIL REFAI, Caltech, NICK BONESTEEL, KUN YANG, FSU, JOEL MOORE, Berkeley — For pure critical spin chains, the scaling of the entanglement entropy of a region of size $L$ with its complement is proportional to $\log L$ with the constant of proportionality being the central charge of the associated conformal field theory. Certain strongly disordered spin chains exhibit critical points with similar $\log L$ scaling. Here we study the disordered golden chain (modeled by fibonacci anyons), and show that the usual random singlet critical point achieved with random antiferromagnetic (AFM) couplings is unstable to ferromagnetic (FM) perturbations. We identify the new mixed FM-AFM fixed point and compute its entanglement entropy scaling.

4:42PM W15.00012 Quantum Ergodicity and the Dynamical Generation of Entanglement in Kicked Coupled Tops, COLLIN TRAIL, VAIBHAV MADHOK, IVAN DEUTSCH, SHOHINI GHOSE, LEIGH NORRIS, ARJENDU PATTANAYAK — We explain how the long-time average dynamically generated entanglement in a Hamiltonian bipartite system is related to the corresponding classical dynamics in the semiclassical limit. Where classical dynamics is chaotic, ergodic mixing leads to the generation of “random quantum states.” These states possess the typical entanglement of a state randomly sampled from the appropriate Hilbert space under the unitarily invariant Haar measure. We exemplify these results using a system of coupled kicked-tops in which entanglement and chaos arise from the same physical effect in contrast to previous studies. We present quantitative predictions of the dynamically generated entanglement, which is influenced by the time symmetries of the system and the structure of the Hilbert space, under a variety of different conditions, and show a close fit to numerical simulations.

5:06PM W15.00014 Few-electron anisotropic quantum dots in low magnetic fields: exact-diagonalization results for excitations, spin configurations, and entanglement

CONSTANTINE YANNOULEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Following earlier studies for $N = 2 - 6$ electrons in anisotropic quantum dots, covering a broad range of confinement anisotropies and strength of inter-electron repulsion, will be presented for zero and low magnetic fields. The excitation spectra are analyzed as a function of the magnetic field and of quantum-dot anisotropy. Analysis of the many-body wave functions through spin-resolved two-point correlations reveals that the electrons tend to localize forming Wigner molecules (WMs). For strong anisotropy, the WMs acquire a linear geometry, and the wave functions with a total spin projection $S_z = (N - 2)/2$ are similar to the strongly entangled $W$ states. For intermediate anisotropy, the WMs exhibit a more complex structure. The degree of entanglement can be quantified through the use of the von Neumann entropy.

1 Supported by the U.S. D.O.E. (FG05-86ER-45234)


Thursday, March 13, 2008 2:30PM - 5:18PM –

Session W16 DBP: Focus Session: Novel Biomedical Techniques

Morial Convention Center 208

2:30PM W16.00001 Novel Radiation Sources Based on Ultra-High-Power Lasers: New Capabilities for Radiology and Radiotherapy

DONALD UMSTADTER, University of Nebraska, Lincoln — As the maximum power level of compact lasers steadily increases, new opportunities are enabled for their use in bio-medicine and medicine. For instance, the Diocles laser at the University of Nebraska, Lincoln, now produces a peak power of 150-terawatts ($1.5 \times 10^{14}$ W) from a table-top-size system. When light at this power level is focused, it can accelerate electrons, and produce quasi-monoeenergetic beams of x-rays, similar to those produced by much larger synchrotron light sources. Such MeV-energy beams create new opportunities in biomedicine, radiology and radiography. Examples to be discussed include structural analysis of bio-molecules, diffraction-enhanced imaging for computed tomography, and radio-sensitization-enhanced radiotherapy. This talk will describe the current status of laser-based x-ray technology, as well as the potential advantages and prospects for their use in medicine.

1 Supported by AFOSR, DARPA, DHS, DOE and NSF.

3:06PM W16.00002 New techniques required to understand the by-stander effect in situ.

RICHARD BRITTEN, Eastern Virginia Medical School — The bystander effect has been known for nearly a century under various names, of which the abscopal effect is probably the most well known. More recently the by-stander effect has received a lot of attention, and various models have been developed to assess the relative importance of the bystander effect in radiation treatment. It is clear that irradiated cells release factors that lead to alterations in the physiology of adjacent irradiated cells, both via inter-cellular junctions and through systemic factors. Most studies that have sought to identify the systemic factors and the cellular mechanisms that are responsible for the bystander effect have by necessity used in vitro systems. The purpose of this presentation is to alert the audience to the various techniques that are available to study the proteomic changes related to the bystander effect in situ. We shall pay attention to the use of MALDI-imaging to track spatial proteomic changes in tissue that have been exposed to microbeams.

3:42PM W16.00003 The Physics of Up-Conversion Nanophosphors for Cancer Treatment

SHUANG-FANG LIM, WILLIAM RYU, Princeton University, ROBERT RIEHN, North Carolina State University, ROBERT AUSTIN, Princeton University — Upconversion phosphors are rare-earth containing crystalline materials which can convert infrared light to visible light (hence the name up-conversion), via excitation of real levels of rare earths. They overcome limitations of current organic fluorophors and quantum dots and have unique properties that enable advanced imaging, drug delivery applications and light-based chemotherapy. The process by which near-IR photons (980 nm) are summed in a rare-earth excitation of real levels of rare earths. They overcome limitations of current organic fluorophors and quantum dots and have unique properties that enable advanced imaging, drug delivery applications and light-based chemotherapy. The purpose of this presentation is to alert the audience to the various techniques that are available to study the proteomic changes related to the bystander effect in situ. We shall pay attention to the use of MALDI-imaging to track spatial proteomic changes in tissue that have been exposed to microbeams.

3:54PM W16.00004 Disposal of Energy by UV-B Sunscreens

THOMAS NORDLUND, Dept. of Physics, Univ. of Alabama/Birmingham, RAJAGOPAL KRISHNAN, Dept. of Dermatol., Univ. of California/SF — Ideal sunscreens absorb dangerous UV light and dispose of the energy safely. “Safe disposal” usually means conversion to heat. However, efficient absorption entails a high radiative rate, which implies high energy-transfer capabilities for Radiology and Radiotherapy. When light at a power level is focused, it can accelerate electrons, and produce quasi-monoeenergetic beams of x-rays, similar to those produced by much larger synchrotron light sources. Such MeV-energy beams create new opportunities in biomedicine, radiology and radiography. Examples to be discussed include structural analysis of bio-molecules, diffraction-enhanced imaging for computed tomography, and radio-sensitization-enhanced radiotherapy. This talk will describe the current status of laser-based x-ray technology, as well as the potential advantages and prospects for their use in medicine.

1 Supported by grants NCI (CA94327) and Univ. of Alabama/Birmingham (Preparing Future Faculty and GAPF fellowship [RK]).

4:06PM W16.00005 Microdosimetry of onidividual cells with microbeam facilities

PAUL GUEYE, Hampton University — This abstract has not been submitted.

4:42PM W16.00006 Dynamical Systems, Cytokine Storms, and Blood Filtration

GLENN FOSTER, ALFRED HUBLER, Center for Complex Systems Research, University of Illinois at Urbana-Champaign, Department of Physics — Various infections and non-infectious diseases can trigger immune cells and the proteins (cytokines) the cells use to communicate with each other to be caught in a positive feedback loop; this “cytokine storm” is frequently fatal. By examining the network of cytokine-immune cell interactions we will illustrate why anti-mediator drugs have been generally ineffective in stopping this feedback. A more effective approach may be to try and reduce interactions by dampening many signals at once by filtering the cytokines out of the blood directly (think dialysis). We will argue that feedback on an out of control nonlinear dynamical system is easier to understand than its normal healthy state and apply filtration to a toy model of immune response.
4:54PM W16.00007 Differentiation of benign epithelia, prostatic intraepithelial neoplasia and, stromal region of prostate biopsies using Raman spectroscopy, HOUBEI DAI, JAGDISH THAKUR, RATNA NAIK, Wayne State University, FAZLUL SARKAR, WAEL SAKR, Karmanos Cancer Research Institute, GREG AINER, ALEX CAO, ABHILASH PANDYA, Wayne State University, VAMAN NAIK, University of Michigan-Dearborn — A pilot study was performed to differentiate the benign epithelium (BE), prostatic intraepithelial neoplasia (PIN) and, stromal regions from deparaffinized prostate needle biopsies using Raman spectroscopy. Raman spectra were collected from six deparaffinized prostate tissues and all the three regions showed different Raman spectral features that may represent unique Raman signatures of these regions. One of the unique features observed in these spectra is that the ratio of the two peak heights at 1449 cm$^{-1}$ and 1338 cm$^{-1}$ is constant with different values for BE and PIN. While the peak at 1338 cm$^{-1}$ is quite weak in the stromal regions. Multivariate statistical methods clearly separated the spectra from three different regions of the tissues into three distinct groups. This study demonstrates the feasibility of using deparaffinized tissue biopsy samples for the diagnostic purpose.

5:06PM W16.00008 Medical Application of the Geant4 Simulation Toolkit, JOSEPH PERL, Stanford Linear Accelerator Center — Geant4 is a toolkit for the simulation of the passage of particles through matter. While Geant4 was originally developed for High Energy Physics (HEP), applications now include Nuclear, Space and Medical Physics. Medical applications of Geant4 in North America and throughout the world have been increasing rapidly due to the overall growth of Monte Carlo use in Medical Physics and the unique qualities of Geant4 as an all-particle code able to handle complex geometry, motion and fields with the flexibility of modern programming and an open and free source code. Work has included characterizing beams and brachytherapy sources, treatment planning, retrospective studies, imaging and validation. This talk will provide an overview of these applications, with a focus on therapy, and will discuss how Geant4 has responded to the specific challenges of moving from HEP to Medical applications.

Thursday, March 13, 2008 2:30PM - 5:06PM — Session W17 DBP: General Biological Physics Morial Convention Center 209

2:30PM W17.00001 Actin-mediated bacterial propagation as dissipative dynamics of F-actin concentration: onset of motion, comet profile, velocity fluctuations, VINCENZO BENZA, Universita’ dell’insubria — Bacterial motion under the action of an actin gel network is described in terms of the F-actin concentration dynamics driven by polymerization, elasticity, and coupling with the bacterium. An explicit formula for the velocity clarifies the role of the different factors contributing to propagation. As regards the onset of motion, we find that smaller ratios of the branching/nucleation rates give rise to an increasingly long buildup time before startup. In the cruise regime the linear growth of the comet length versus velocity is analytically shown and numerically verified; as the length increases the concentration maximum decreases. Both features have been observed in kinematics experiments [1]. By expanding our previous work [2], we show that a larger elasticity modulus makes a larger velocity but with a smaller contribution from the interface polymerization. At steady state we find two regimes: constant velocity when the branching rate dominates over the nucleation rate, intermittent velocity when the two rates are comparable. In this case the concentration profile does not display macroscopic fluctuations, but the distance of its maximum from the bacterium surface oscillates: this behavior has its counterpart in the intermittency of the cruise velocity.


2:42PM W17.00002 The contraction of Vorticella in different Ca concentration solutions, DEEPENDRA KANTHA, DAVID VAN WINKLE, Department of Physics, Florida State University and Center for Materials Research and Technology (MARTECH) — The contraction of the stalk of *Vorticella Convallaria* was studied in media with different concentrations of calcium ion solution. Seven solutions were prepared by adding different amounts of CaCl$_2$ in the range of 0.001M to 0.004M EGTA, 0.1M KCl and 0.02M MOPS. The pH values of the solutions were maintained between 6.7 and 6.9. The contractions were recorded as images (image sequences) by a Phantom V5 camera (Vision Research) on a bright field microscope with 20X objective, with the image resolution of 256 $\times$ 128 pixels at 7000 pictures per second. The change in length of stalk as a function of time was analyzed to compute velocity, acceleration, force and force coefficient. The apparent force coefficient increases linearly with time until the whole stalk is maintained between 6.7 and 6.9. The contractions were recorded as cines (image sequences) by a Phantom V5 camera (Vision Research) on a bright field microscope with 20X objective, with the image resolution of 256 $\times$ 128 pixels at 7000 pictures per second. The change in length of stalk as a function of time was analyzed to compute velocity, acceleration, force and force coefficient. The apparent force coefficient increases linearly with time until the whole stalk is contracting. Considering time dependence of force coefficient, the contracting length is modeled as:

$$L(t) = \frac{L_0}{2} \left[ \left(1 + \frac{C_1}{A} \right) \exp \left( -\frac{C + A t}{2m} \right) + \left(1 - \frac{C_1}{A} \right) \exp \left( -\frac{C - A t}{2m} \right) \right]$$

Where $L_0$ is initial contractile length, $C = 6\eta r$, $A = \sqrt{C^2 - 4m K(t)}$, $\eta$ is coefficient of viscosity, $m$ is mass and $r$ is radius of zooid.

2:54PM W17.00003 Kinetics of Multideterminate Ligand Binding, IGOR GONCHARENKO, MIKE COLVIN, AJAY GOPINATHAN, University of California, Merced — The binding of multivalent ligands to cell surface receptors is an inherent feature of many biological processes and is technologically important in designing drug delivery systems. We analyze the binding and unbinding kinetics of a multi-armed ligand to normal and cancerous cells in terms of the residence time. By mapping the problem to a first passage time solution of the dynamics described by a multi-dimensional Fokker-Plank equation we are able to derive the residence times of the ligands on the cell surface as a function of the number of arms, binding affinity, polymer statistics of the linker arms as well as density, distribution and types of receptor binding sites. Our results point towards ways of optimizing these parameters so as to selectively target diseased cells with specially designed ligands that are capable of drug delivery. Our results also shed light on the recognition and response kinetics of a variety of cell types with specific functions that are triggered by the binding of surface receptors to exogenous ligands.

3:06PM W17.00004 Single cell visualization of DNA repair in vivo, AZADEH SAMADANI, BrandeisUniversity, AMY ROWAT, SEAS, Harvard University, JENNIFER MAKRIDAKIS, JAMES HABER, Brandeis University — The creation of a DNA double-strand-break constitutes the most dangerous type of DNA damage. Efficient response to DNA damage may lead to hypersensitivity to cellular stressors, susceptibility to genomic defects and resistance to apoptosis, which can lead to cancer. Current research on DNA repair has enabled numerous breakthroughs in our understanding of the DNA repair mechanisms at the population level. However, similar understanding at the level of single cells has been lacking mainly because of two reasons: 1) population level measurements do not visualize the repair process and therefore the exact mechanism by which the donor and recipient sequences are brought together is not well understood. 2) they are only sensitive to the mean of a distribution and usually hide the cell-to-cell variability of the repair processes. In my lab we utilize a multidisciplinary approach to address specific aspects of the DNA repair at the single cell level. By tagging several locations on DNA, its dynamic is visualized. Furthermore the exact timing of the repair process is measured. In our experiments, individual cells are followed over long periods of time and many cellular generations in a microfluidic device, in which a precise control of the microenvironment of the cells is possible.
3:18PM W17.00005 Current reversal in collective rocking ratchets induces by ground state instability

We thanks Spanish Ministerio Educacion y Ciencia grants NAN04-09087, FIS05-07392.

3:30PM W17.00006 A Mathematical Exploration of MAP Kinase Behavior


3:42PM W17.00007 Electric field control of the cell orientation

1. JOSE L. VICENT, LUIS DINIS, ELVIRA M. GONZALEZ, Universidad Complutense, 28040 Madrid, Spain, JOSE V. ANGUIITA, Instituto Microelectronica, CSIC, 28760 Madrid, Spain, JUAN M.R. PARRONDO, Universidad Complutense, 28040 Madrid, Spain — A collective mechanism for current reversal in rocking ratchets is proposed. The mechanism is based on a two-dimensional instability of the ground state of the system. We illustrate our results with numerical simulations and experiments using the dynamics properties of superconducting vortex lattice in Nb superconducting films fabricated on top of Si substrates with array of asymmetric nanodefects.

This work was supported through MDACC start-up funds.

3:54PM W17.00008 X-ray studies of crystal transformation in dehydrating trehalose

1. This work is supported by the National Science Foundation.
4:42 PM W17.00012 AC electrokinetics of dense inhomogeneous biological cells suspensions under nonuniform applied fields, K.L. CHAN, The Chinese University of Hong Kong, J.P. HUANG, Fudan University, K.W. YU, The Chinese University of Hong Kong — When a biological cell is placed in a nonuniform AC (or DC) electric field, force would be induced because of the interaction between the induced electric dipole moment of the particle and the external electric field. This phenomenon is called dielectrophoresis (DEP). [1] In this study a new method is proposed to handle biological cells with arbitrary permittivity and conductivity profiles, and determine the importance of multiple effect as compared with the approximate point dipole calculation [2], which is valid if the external field is homogeneous. In real situations, cells often possess arbitrary graded profiles and the study of higher multipole effects can lead to a better understanding. We also extend the calculation to dense cells suspensions by the effective medium theories [3]. The study reveals significant effects on the DEP due to higher concentration.


4:54 PM W17.00013 Folding of Pollen Grains, ELENI KATIFORI, Department of Physics, Harvard University, Cambridge MA, SILAS ALBEN, School of Mathematics, Georgia Institute of Technology, Atlanta, GA, ENRIQUE CERDA, Departamento de Física, Universidad de Santiago, Chile, DAVID NELSON, Department of Physics, Harvard University, JACQUES DUMAIS, Department of Organismic and Evolutionary Biology, Harvard University — At dehiscence, which occurs when the anther reaches maturity and opens, pollen grains dehydrate and their volume is reduced. The pollen wall deforms to accommodate the volume loss, and the deformation pathway depends on the initial turgid pollen grain geometry and the mechanical properties of the pollen wall. We demonstrate, using both experimental and theoretical approaches, that the design of the apertures (areas on the pollen wall where the stretching and the bending modulus are reduced) is critical for controlling the folding pattern, and ensures the pollen grain viability. An excellent fit to the experiments is obtained using a discretized version of the theory of thin elastic shells.

Thursday, March 13, 2008 2:30PM - 5:18PM –
Session W18 DPOLY DBP: Focus Session: Dynamics of Nucleic Acid-Protein Interactions
Morial Convention Center 210

2:30PM W18.00001 Single-Molecule Dynamics of a DNA Aptamer Targeting VEGF Protein, CHRISTY LANDES, University of Houston — Single-molecule fluorescence resonance energy transfer (SMFRET) and SMFRET autocorrelation analysis were used to examine structural fluctuations in a DNA aptamer that binds and exhibits inhibition activity towards the vascular endothelial growth factor (VEGF) protein, a protein that is involved in macular degeneration. The aptamer’s most stable conformation contains 4 Watson-Crick base pairs, resulting in only a shallow negative potential relative to the unfolded state. The weakly stable folded state and the manifold of unfolded structures quickly interconvert. In contrast, in the presence of the VEGF target, the aptamer folding rate constant decreases and the fluctuations in both the unfolded and folded states decrease in frequency, but are not eliminated. A possible relationship between activity and aptamer flexibility is discussed.

3:06PM W18.00002 Thermal Disorder Effect on the DNA Electronic Structure, ALEXANDER BALEFF, Duke University, ELIZABETH HATCHER, University of Maryland, Baltimore, SHAHAR KEINAN, RAVINDRA VENKATRAMANI, DAVID BERATAN, Duke University — We address the effect of the thermal dynamics of DNA structure on the energy and localization of the DNA electronic orbitals. Structural ensembles are generated for several DNA sequences by molecular dynamics simulations employing CHARMM and AMBER force fields. In the shortest sequences studied (CATG, GAAG, CAGT, GACG), the highest occupied molecular orbitals (HOMOs) expectedly reside on the guanines (Gs), yet in a significant number of the structures the orbitals are observed to be delocalized between the Gs and the bridging adenines (As). Adding more Gs to the ends of the sequence expectedly shifts the orbitals toward the G clusters, yet the amount of orbital delocalization to the bridge is still significant. These observations suggest that a) contrary to the predominant view in the field, G-to-A thermal hopping may contribute significantly to the charge transfer in DNA even in the short-distance range, and b) the contribution of DNA structural fluctuations to triggering the charge transfer is as significant as that resulting from the ion gating mechanism.

3:18PM W18.00003 Thermodynamic Restriction on Evolutionary Optimization of Transcription Factor Proteins, ALEXANDER GROSBERG, LONGHUA HU, University of Minnesota, ROBIJN BRUINISMA, University of California Los Angeles — Conformational fluctuations are believed to play an important role in the process by which transcription factor proteins locate and bind their target site on the genome of a bacterium. Using a simple model, we show that the binding time can be minimized, under selective pressure, by adjusting the spectrum of conformational states so that the fraction of time spent in more mobile conformations is matched with the target recognition rate. The associated optimal binding time is then within an order of magnitude of the limiting binding time imposed by thermodynamics, corresponding to an idealized protein with instant target recognition. Thus, we claim that it is possible for the overall binding rate of a transcription factor to approach the theoretical limiting value but only by a suitable choice of energy spectrum of conformational sub-states, and only if the dimensionless binding rate is of the order of one, or larger than one, where dimensionless binding rate is determined as the product of binding rate and the average time spent by the protein on one DNA base pair in one turn of 1D sliding along DNA. Numerical estimates suggest that typical bacteria operate in this regime of optimized conformational fluctuations.

3:30PM W18.00004 Electron affinities of nucleobases, glycine and their complexes1, ED S. CHEN, Baylor College of Medicine, EDWARD C. CHEN, The Wentworth Foundation — The electron affinities of adenine, guanine, and the amino acids except for glycine have not been measured in the gas phase. New valence state electron affinities of the subject molecules are reported from reduction potentials and literature anion photoelectron spectra. These are supported by quantum mechanical calculations. Multiple negative ion potential energy curves are calculated to consolidate reduction potentials, electron impact spectra in helium nanodroplets, negative ion mass spectra, electron transmission spectra, electron spin resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5). Adenine: thymine 1.40(5) eV. Excited dipole resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5). Adenine: thymine 1.40(5) eV. Excited dipole resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5) Adenine: thymine 1.40(5) eV. Excited dipole resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5). Adenine: thymine 1.40(5) eV. Excited dipole resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5) Adenine: thymine 1.40(5) eV. Excited dipole resonance data for DNA, A method of measuring negative valence state electron affinities using ESR data is proposed. The adiabatic electron affinities are: in eV Adenine, 1.08(5), Guanine, 1.65(10), Cytosine, 1.04(5), Thymine, 0.98(5), Uracil, 0.99(5), Glycine, 0.50(5).

1The Wentworth Foundation

3:42PM W18.00005 Chemical physics of DNA packaging in a nucleosome core particle, ANDREW SPAKOWITZ, BARIZ SUDHANSHU, Stanford University — The fundamental unit of packaged DNA, the nucleosome core particle, contains 146 base pairs of DNA wrapped 1.7 times around a cationic protein complex called the histone octamer. A string of nucleosomes is organized into higher-order structures at the sites of gene expression. The nucleosome’s most stable conformation contains 4 Watson-Crick base pairs, resulting in only a shallow negative potential relative to the unfolded state. We proceed to construct a free energy surface to predict the dynamic response in tension. We employ the wormlike chain model to describe the DNA strand as a thermally fluctuating polymer chain. The chain adsorbs on a spool that accommodates the volume loss, and the deformation pathway depends on the initial turgid pollen grain geometry and the mechanical properties of the pollen wall. We demonstrate, using both experimental and theoretical approaches, that the design of the apertures (areas on the pollen wall where the stretching and the bending modulus are reduced) is critical for controlling the folding pattern, and ensures the pollen grain viability. An excellent fit to the experiments is obtained using a discretized version of the theory of thin elastic shells.
we discuss how different patterns of nucleosome positions, periodic or random, could either facilitate or suppress heterochromatin stability and formation. The role nucleosome positioning might play in the formation of heterochromatin, a compact form of DNA generically responsible for gene silencing. In particular, the octamer experience a sequence dependent energy landscape due to the variation in DNA bend stiffness with sequence composition. In this talk, we consider the physics and astronomy of heterochromatin.

3:54PM W18.00006 DNA analysis in polymer nanofluidic devices

Partial support from EC funded project NaPa (Contract no. NMP4-CT-2003-500120) is acknowledged.

4:06PM W18.00007 Separation of long DNA molecules through cleavage of hydrogen bonds under a stretching force

This work is supported by NSF under Agreement No. 0112050.

4:18PM W18.00008 Self-organized DNA/F-actin gels: entangled networks of nematic domains with tunable density

This work was supported in part by the NSF DMR-0409769, NIH 1R21DK6843-01, the Cystic Fibrosis Foundation, and the Institute for Complex Adaptive Matter.

4:30PM W18.00009 Histone code or not? Combinatorial pattern analyses of histone modifications

1This work is supported by NSF under Agreement No. 0112050.

4:42PM W18.00010 Changes of histone modification landscape in cell differentiation

5:06PM W18.00012 Nucleosome Positioning and Epigenetics

5:28PM W18.00013 Defects and doping of semiconductors
The role of nitrogen vacancies and hydrogen in conductivity of InN.

Anderson Janotti, Chris G. Van de Walle, Materials Department, University of California, Santa Barbara, CA 93106 — Using first-principles methods we investigate the electronic properties and stability of the nitrogen vacancy and monatomic hydrogen in InN. We find that nitrogen vacancies act as shallow donors, but they have high formation energies in n-type InN. Therefore, N vacancies are unlikely to cause the observed unintentional n-type conductivity in as-grown InN. Hydrogen can occupy interstitial as well as substitutional sites in InN. Interstitial hydrogen has low formation energy, is stable in the bond-center configuration, and acts exclusively as a shallow donor (H⁺). The calculated frequency of the H-N stretching mode is 3050 cm⁻¹. Hydrogen can also substitute for nitrogen in InN, bonding equally to the four In nearest neighbors in a multicenter-bond configuration [1]. Substitutional hydrogen also has low formation energy and, counterintuitively, forms a double-donor center. Our results suggest that hydrogenic hydrogen is a plausible cause of the unintentional n-type conductivity that is almost universally observed in as-grown InN.

3:42PM W19.00007 Electrical activation studies of Al\textsubscript{0.4}Ga\textsubscript{0.6}N and Al\textsubscript{0.5}Ga\textsubscript{0.5}N implanted with silicon for n-type doping. ELIZABETH MOORE, YUNG KEE YEO, Air Force Institute of Technology, MEE-YI RYU, Kangwon National University, ROBERT HENGELOTH, Air Force Institute of Technology — A systematic electrical study of Si-implanted Al\textsubscript{0.4}Ga\textsubscript{0.6}N with Al concentrations of 40 and 50\% grown on sapphire substrates by MEMOCVD has been made as a function of ion dose and anneal temperature. The silicon ions were implanted at 200 keV with doses from 1x10\textsuperscript{14} to 1x10\textsuperscript{16} cm\textsuperscript{-2} at room temperature. The samples were proximity cap annealed from 1150 to 1350 °C for 20 minutes in a nitrogen environment. Hall-effect measurements were made from 10 to 700 K and cathodoluminescence measurements were taken at 7 K. Electrical activations of nearly 100\% were obtained for the Al\textsubscript{0.4}Ga\textsubscript{0.6}N:Si after annealing at 1350 °C for 20 minutes for doses of 1x10\textsuperscript{15} and 5x10\textsuperscript{15} cm\textsuperscript{-2} and after annealing at 1200 °C for 20 minutes for the dose of 1x10\textsuperscript{15} cm\textsuperscript{-2}. The Al\textsubscript{0.5}Ga\textsubscript{0.5}N:Si also had high activations of nearly 100\% for the two lower doses after annealing at 1300 °C for 20 minutes, while for a dose of 1x10\textsuperscript{15} cm\textsuperscript{-2}, an activation of 66\% was obtained after the same annealing treatment. The highest room temperature mobility for the Al\textsubscript{0.4}Ga\textsubscript{0.6}N and Al\textsubscript{0.5}Ga\textsubscript{0.5}N samples is 61 and 55 cm\textsuperscript{2}/V·s, respectively for the samples annealed at 1350 °C for 20 minutes. CL spectra support the electrical results in determining the optimal annealing conditions.

3:54PM W19.00008 Effects of Dopants and Annealing on the Structure and Electronic properties of GaAsN\textsuperscript{1}. YU JIN, MATTHEW REASON, HAILING CHEN, CAGLIYAN KURDACK, RACHEL GOLDMAN, University of Michigan — In this work, we investigate the effects of different n-type dopants and rapid thermal annealing (RTA) on the structure and electronic properties of GaAsN bulk-like films grown by molecular beam epitaxy. For as-grown GaAs:N:Si and GaAsTe films, similar free carrier densities (n) and electron mobilities (μ) are observed. However, after post-growth RTA, a substantial increase in both n and μ is observed in the GaAsTe films, with negligible change in those of the GaAs:N:Si films. Apparently, RTA reduces the concentration of N-related trapping and scattering centers in GaAsTe. On the other hand, the annealing process enhances the diffusion of Si, presumably leading to the formation of additional N\textsubscript{As}–Si\textsubscript{Si} defect complexes. For both GaAsTe and GaAsSi films, x-ray rocking curves reveal reduced lattice parameters following annealing, suggesting a decrease in the interstitial [N], which leads to the improvement in electronic properties for the GaAsTe films. In the case of GaAsSi, the reduction in interstitial [N] is presumably balanced by an increase in the density of N\textsubscript{As}–Si\textsubscript{Si} defect complexes. The effect of dopants and annealing on the structure and electronic properties of InGaAsN will also be discussed.

1Supported by NSF-FRG, grant # DMR-0660406, monitored by L. Hess.

4:06PM W19.00009 Bismuth related transitions in the electronic properties of high quality dilute GaAs\textsubscript{1−xBi\textsubscript{x}}. LEKHNATH BHUSAL, DENIS KARAIASKAJ, RYAN FRANCE, AARON PTAK, ANGELO MASCARENHAS, National Renewable Energy Laboratory, 1617 Cole Blvd, Golden CO-80401, TOM TIEDJE, AMPLE, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T 1Z4 — In this work we will present the electronic and optical properties of dilute GaAs\textsubscript{1−xBi\textsubscript{x}} epilayers for the range of samples with concentration up to ~3\%. Variation of fundamental band gap (E\textsubscript{G}) and the transition from the spin-orbit split off valance band (E\textsubscript{V} + Δ) using the contactless modulated electroreflectance will be presented as a function of temperature (77-300K) and Bi concentrations. We will also discuss the isoelectronic codoping of Bi and nitrogen, as the excellent quality of GaAsBi samples presented in the work opens the path for the codoping of Bi with N to improve the electronic properties of dilute nitride III-V alloys.

We acknowledge the financial support of the Department of Energy, Office of Sciences, Basic Energy Sciences, and Division of Material Sciences.

4:18PM W19.00010 A defect relaxation model for the carbon vacancy in SiC. JAMIYANAA DASHDORJ, MARY ELLEN ZVANUT, Physics Department, University of Alabama at Birmingham — Deep level intrinsic defects in high purity semi-insulating SiC play an important role in electrical compensation necessary to achieve high resistivity. We use a constant light intensity approach to steady-state photo-electron paramagnetic resonance (EPR) and time-dependent photo-EPR to study the ionization cross sections and relaxation energies of the well-studied defect, the positively charged carbon vacancy, V\textsuperscript{+}C. As-grown 4H-SiC samples with room temperature resistivity of 10\textsuperscript{10} Ohm-cm were studied at 4 K and 80 K. The shape of the absorption curve for V\textsuperscript{+}C, as revealed by the steady state measurements, has a peak at 2.3 eV and photo-threshold at 1.8 eV. We interpret the difference between these two values as a structural relaxation upon release of an electron from the defect to conduction band. Consistently, preliminary time-dependent measurements reveal a Franck-Condon transition at 2.3 eV for release of an electron from the defect to the conduction band, and a second Franck-Condon transition at an energy greater than 1.3 eV for capture of electron at the defect from the valence band. The difference of no more than 1 eV may be interpreted as a relaxation energy, consistent with the interpretation of steady-state data. The details of the experimental approach and the formulation of the relaxation model will be presented.

4:30PM W19.00011 Direct Imaging of Point Defect Configurations for Au Atoms Inside Si Nanowires\textsuperscript{1}. K. VAN BENTHEM, S.H. OH, A.Y. BORISEVICH, W. LUO, Oak Ridge National Laboratory, P. WERNER, N.D. ZAKHAROV, MPI for Microstructure Physics, S.T. PANTELIDES, Vanderbilt University, S.J. PENNYCOOK, Oak Ridge National Laboratory — Aberration-corrected scanning transmission electron microscopy (STEM) was used to directly image individual Au atom configurations inside Si nanowires grown by Au-catalyzed vapor-liquid-solid molecular beam epitaxy. A three-dimensional analysis of the nanowire microstructure revealed Au atom concentrations five orders of magnitude higher than equilibrium values in bulk silicon. Three distinct interstitial Au atom configurations were identified in addition to the substitutional configuration. The stability of the observed point defect configurations was further investigated by density-functional theory. The observed configurations are in excellent agreement with theory. However, comparison of the number densities of the various configurations with the calculated formation energies indicates an effective temperature of approximately 1000 degrees centigrade suggesting significant beam-induced atomic diffusion.

This work was supported by the Office of Basic Energy Sciences, DMSE (AYB, SJP) and DSUF (AYB, KvB), an NSF-NIRT project (SHO), and the European Union (NDZ).

4:42PM W19.00012 Ni doping of semiconducting boron carbide\textsuperscript{1}. S. ADENWALLA, JING LIU, NINA HONG, Physics and Astronomy, Univ. of Nebraska-Lincoln — Semiconducting boron carbide (BC) is intrinsically p-type. The addition of Ni has been shown to dope it n-type. I-V measurements on Ni doped BC on both p- and n-type Si (1x10\textsuperscript{15} cm\textsuperscript{-3} and 4.5x10\textsuperscript{15} cm\textsuperscript{-3}) indicate changes in the doping level with increasing Ni concentration. At the highest dopant level, Ni doped BC on n-type Si showed n-n+ diode characteristics. The change of doping concentration was confirmed by the built-in potential increase from 0.1 V in the low Ni doped p-n diode to 1.2 V in the high Ni-doped p-n diode as well as by measurements of the reverse saturation current. The addition of Ni does not lead to significant structural changes in the BC as measured by x-ray diffraction. X-ray fluorescence data indicate an upper bound of 2 ppm for the Ni concentration. Using these results homojunction p-n diodes were fabricated from layers of undoped p-type BC and Ni doped n-type BC and characterized by I-V and capacitance-voltage (C-V) measurement. Homojunction devices are shown to be especially promising for thermal neutron detection.

\textsuperscript{1}Funded by NSF-0725881 and NASA NNG05GM89G.
4:54PM W19.00013 First principles investigations into alkali intercalation of hexagonal boron nitride. BAHADIR ALTINTAS, Abant Izzet Baysal University, Department of Chemistry, CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University, Department of Chemistry — Although hexagonal boron nitride (hBN) is quite similar to graphite structurally, it has been very difficult to obtain any intercalation compound of hBN while there are hundreds of graphite intercalation compounds. We have investigated the possible intercalation of hBN by alkali atoms in the density functional theory framework by using pseudopotentials and plane-wave basis. The structural, electronic and lattice dynamical properties of hypothetical hBN analogues of LiC$_3$, LiC$_6$, K$_5$C$_6$, Cs$_5$C$_6$, Ca$_5$C$_6$ are calculated. We have found that although the electronic structure, band structure and free surface of alkali intercalated hBN is very similar to that of alkali intercalated graphite, the lattice dynamics show a set of negative frequency modes which indicate that alkali-intercalated hBN is not stable.

5:06PM W19.00014 Effects of point defects on the electrical properties of aluminum antimonide: a first principles investigation. VINCENZO LORDI, DANIEL ÅBERG, PAUL ERHART, Lawrence Livermore Lab — A first principles study is conducted on the effects of point defects on the electrical properties of bulk AI$_3$Sb, a material of interest for room temperature gamma radiation detection. Detailed calculations were performed for all native defects, including vacancies, antisites, interstitials, and split interstitials, and also for a variety of impurities (H, C, Si, Ge, Sn, P, O, S, Se, Te). Formation energies of each defect in different charge states were calculated to determine the equilibrium defect density and net carrier density. Carrier scattering rates for each defect were calculated using perturbation theory to determine the effects on electron and hole transport. The most detrimental, as well as innocuous, defects were identified. Relative solubilities of the impurities were examined along with their scattering rates to find efficient dopants that minimize mobility degradation. Finally, carrier trapping cross sections and energy levels were calculated to study the role of each defect in deep level trapping.

1Prepared by LLNL under Contract DE-AC52-07NA27344.

Thursday, March 13, 2008 2:30PM - 5:18PM Session W20 DCMP: Oxide Surfaces, Interfaces and Thin Films Morial Convention Center 212

2:30PM W20.00001 Electronic structure of epitaxial CrO$_2$(100) and CrO$_2$(110) films. C. A. VENTRICE JR, H. GEISLER, Texas State Univ., D. R. BORST, Univ. of New Orleans, G. X. MIAO, A. GUPTA, Univ. of Alabama — Half-metallic ferromagnets are conducting solids whose conduction electrons undergo magnetic ordering with a spin polarization of 100% at 0 K. Although CrO$_2$ is predicted to be a half-metallic ferromagnet, previous attempts to make devices using CrO$_2$ have resulted in a degradation of performance instead of an enhancement. Using ultra-violet photoluminescence spectroscopy at the CAMD synchrotron, we have measured the electronic properties of epitaxial CrO$_2$(110)/TiO$_2$(110) and CrO$_2$(100)/TiO$_2$(100) surfaces grown using a CrO$_2$ precursor. Clean, stoichiometric CrO$_2$ surfaces have been prepared either by exposure to white light, which desorbs OH groups from the surface, or by sputtering and annealing in O$_2$. The measurements of the CrO$_2$ surfaces show no emission at E$_F$, after sputtering and annealing the surfaces in oxygen. However, the white light prepared surfaces show a small density of states at E$_F$. Photon energy dependent photoemission experiments show no increase in the density of states at E$_F$ as the photon energy is lowered from 50 eV to 15 eV, which increases the bulk sensitivity of these measurements. These results indicate that CrO$_2$ behaves more like a semi-metal than a half-metal and that surface disorder can induce a semi-metal to semiconductor transition at its surfaces.

2:42PM W20.00002 Variation of Growth Mode with Orientation for Epitaxial CrO$_2$ Films. KRISHNA CHETRY, HUNTER SIMS, WILLIAM BUTLER, ARUN GUPTA, University of Alabama — Thin films of CrO$_2$ have been grown epitaxially on (110) and (100) oriented TiO$_2$ substrates. CrO$_2$(100) films grow in a layer by layer mode, while an island growth mode is observed for CrO$_2$(110) films as confirmed from atomic force microscopy (AFM) studies. To better understand the differences in the growth mode, we have performed first principles-based calculations using density functional theory implemented within the VASP code to study the surface and interface energies of CrO$_2$(100), (110), TiO$_2$(100) and (110) systems. For these calculations a periodic repeating slab geometry is used with a sufficient vacuum width and thickness to converge the surface energy within 0.01 meV/Å$^2$. From our calculations we find that $\sigma_{\text{CrO}_2}/\sigma_{\text{TiO}_2} > \chi_{\text{CrO}_2} + \gamma_{\text{CrO}_2}$, where $\sigma$ is the surface energy and $\gamma$ is the interfacial energy between CrO$_2$ and TiO$_2$ system. This result is consistent with the island growth mode observed experimentally for (110) orientation. For the case of (110) orientation also we find that $\sigma_{\text{CrO}_2} < \chi_{\text{CrO}_2} + \gamma$, which does not match with our experimental results. We speculate that formation of some oxygen deficient phase of chromium oxide in the very first monolayer, which then gets converted to CrO$_2$ by accepting oxygen from the second layer, favors the layer-by-layer growth mode in CrO$_2$(100).

2:54PM W20.00003 Self-Assembled Epitaxial Multiferroic Nanocomposite Films Prepared by Polymer-Assisted Deposition. HONGMEI LUO, HAO YANG, EVE BAUER, T. MARK MCCLESKEY, ANTHONY K. BURRELL, QUANXI JIA, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — Multiferroic materials, which show simultaneous electric and magnetic ordering, have attracted considerable interest recently due to their unusual physical properties and potential device applications. Here we demonstrate that a cost-effective chemical solution approach of polymer-assisted deposition (PAD) is a very promising technique to grow self-assembled epitaxial multiferroic nanocomposite thin films: such as BaTiO$_3$-NiFe$_2$O$_4$ films grown on (001)-oriented LaAlO$_3$ substrate. X-ray diffraction (XRD), atomic force microscopy (AFM) and high resolution transmission electron microscopy (HRTEM) analyses show clear epitaxial relationship between the two phases and the substrate. The ferroelectric BaTiO$_3$ grains are embedded in the ferrimagnetic spinel NiFe$_2$O$_4$ matrix. The composite films exhibit both ferroelectric and ferrimagnetic properties. The structure and properties will be discussed and compared with the nanocomposite films prepared by pulsed-laser deposition (PLD) method.

1This work was supported by LDRD Project at LANL.

3:06PM W20.00004 Structural and electrical properties of self-assembled (BiFeO$_3$)$_{0.5}$(Sm$_2$O$_3$)$_{0.5}$ nanocomposite films. HAO YANG, Superconductivity Technology Center, Los Alamos National Laboratory, H. WANG, Department of Electrical and Computer Engineering, Texas A&M University, J.L. MACMANUS-DRISCOLL, Department of Materials Science and Metallurgy, University of Cambridge, Q.X, JIA, Superconductivity Technology Center, Los Alamos National Laboratory — Self-assembled (BiFeO$_3$)$_{0.5}$(Sm$_2$O$_3$)$_{0.5}$ nanocomposite films were deposited on (001) SrTiO$_3$ and Nb-doped SrTiO$_3$ substrates by pulsed laser deposition using a single uniformly mixed target. Analysis from both high-resolution X-ray diffraction and transmission electron microscopy revealed self-assembled epitaxial two-phase BiFeO$_3$ (BFO) and Sm$_2$O$_3$ (SmO) composites in nanoscale. The BFO and SmO domains have grown alternately and vertically aligned with average column size of 10 nm. The dielectric properties of BFO:SmO nanocomposite films were investigated and compared with those of pure BFO and SmO thin films. The dielectric constant of the nanocomposites can be well described by a parallel connection of two individual dielectrics of BFO and SmO. On the other hand, the dielectric loss of nanocomposite films is lower than the theoretical value from such a parallel connection model. This might originate from the reduction of leakage current density of BFO phase in nanocomposite film due to the much larger interfacial area and the strong out-of-plane strain of BFO column.
3:18PM W20.00005 Checkerboard pattern formation in spinel oxide films. TOSHIHITO ASADA, NISSAN ARC, LTD., Rutgers Univ., YOICHI HOBIE, SOONYONG PARK, NARA LEE, Rutgers Univ. — A few-nanometer-size columnar superlattice with a checkerboard (CB) structure has been fabricated by harnessing Jahn-Teller structural distortions. In this talk, we will discuss the growth mechanism of the CB structures in thin films, obtained from the results of our transmission electron microscopy. Ionic diffusion for the phase separation occurs along the direction parallel to the twin boundaries in the high-temperature tetragonal phase. This anisotropic phase separation suggests the importance of the strain associated with the twin structure in the high-temperature tetragonal phase. 1. S. Yeo et al., Appl. Phys. Lett. 89, 233120 (2006). 2. C. L. Zhang et al., Appl. Phys. Lett. 90, 133123 (2007).

3:30PM W20.00006 Thermal Stability of Epitaxial SrTiO$_3$ Thin Films on Si (001). C. YONG, RAJESWARI KOLAGANI, S. ADHIKARI, Towson U, W. VANDERLINDE, Lab for Physical Sciences, L. SALAMANCA-RIBA, U of Maryland, Y. LIANG, Motorola Labs, S. FRIEDRICH, Lawrence Livermore National Lab — Epitaxial SrTiO$_3$ on Si(001) is important for application as a high $\kappa$ (Kappa) gate oxide and is also suitable as a buffer layer for the subsequent growth of other perovskite oxide thin films to enable integration of perovskite oxide functionality with Si. For the latter application, the thermal stability of the interface structure in epitaxial SrTiO$_3$ thin films grown by molecular-beam epitaxy on Si (001) becomes a key issue since most of the perovskite layers are grown at relatively high temperatures (750-850 °C). SrTiO$_3$ and Si are intrinsically thermodynamically unstable in proximity to each other, with some reduction of the $\text{TiO}_2$ and oxidation of the Si to be expected. We have used x-ray diffraction and micro-analytical techniques including optical microscopy, atomic force microscopy (AFM), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to study the thermal stability of epitaxial SrTiO$_3$ thin films grown by molecular beam epitaxy (MBE) on Si (001). Elemental composition of the amorphous interface layer (AIL) and of the epitaxial SrTiO$_3$ film will change during various thermal treatments and gas environments encountered in the subsequent growth of other oxide layers.

3:42PM W20.00007 Design and characterization of Pb(Zr,Ti)O$_3$ /CoFe$_2$O$_4$ Multilayer epitaxial thin films. NORA ORTEGA, ASHOK KUMAR, RAM KATIYAR, University of Puerto Rico — Multiferroics are a novel class of next generation multifunctional materials. Intensive research is being pursued towards the development of materials with high magnetoelectric (ME) coupling. We have fabricated epitaxial Pb(Zr,Ti)$_x$CoFe$_2$O$_4$ (PZT-CFO) multilayer (ML) thin films using pulsed laser deposition on (001) oriented lattice matched SrRuO$_3$/SrTiO$_3$ (SRO/STO) substrates. X-ray diffraction and Raman analysis revealed that PZT and CFO were in the perovskite and spinel phases respectively, in the multilayer thin films having high crystalline quality. The TEM and STEM line scan of the multilayer thin films showed that the layered structure was maintained. Magnetic hysteresis loop showed the ferromagnetic behavior of ML structure, which is independent of the ML configuration. Ferroelectric properties and temperature dependence magnetization will be discussed.

3:54PM W20.00008 Epitaxial oxide heterostructures on silicon. AGHAM POсадAS, J.W. REINER, F.J. WALKER, C.H. AHN. Yale University — Silicon-based MOSFETs will soon be limited by the large off-state leakage current due to tunneling through the 1 nm thick silicon oxynitride gate dielectric layer. One solution is to replace the silicon oxynitride with a high dielectric constant material, such as LaAlO$_3$, which has a relatively large dielectric constant of 24 and band gap of 5.6 eV. We have recently grown LaAlO$_3$ epitaxially on silicon via a transition layer consisting of SrTiO$_3$. The thickness of this SrTiO$_3$ layer is kept between 2 and 5 unit cells because of considerations of epitaxial strain and the atomic-scale interactions between the perovskite structure and the silicon substrate. The oxide heterostructures show atomically abrupt interfaces and dielectric constants close to the bulk value of LaAlO$_3$. Frequency and voltage dependent measurements of the complex impedance of the as-grown oxide heterostructures show a pinned Fermi level and a high density of interface states. Annealing at temperatures in wet oxygen shows that the Fermi level can be unpinned, with a greatly reduced density of interface states.

4:06PM W20.00009 Pulsed Laser Deposition of SrTiO$_3$ Thin Films: Time-Resolved X-ray Studies$^1$. JOEL BROCK, GOKHAN ARIKAN, JOHN FERGUSON, ARTHUR WOLL, Cornell University — X-ray scattering and reflectivity have been used to measure the static atomic structure of surfaces and interfaces for several decades. Modern synchrotron x-ray facilities now deliver sufficient flux to make time-resolved measurements on a wide variety of evolving surface and interface systems feasible. Here, we use time-resolved x-ray diffuse scattering studies of Pulsed Laser Deposition (PLD) of SrTiO$_3$ films on the (001) surface of SrTiO$_3$ to obtain detailed insight into the fundamental, atomic-scale growth mechanism. The data demonstrate that during-layer-by-layer growth, islands are nucleated during the 1$^{st}$ pulse. The size of the pulse determines the nucleation density. During and in between subsequent pulses, the islands coarsen and coalesce. Line shape analysis of the diffuse scattering reveals that adatom capture occurs at the same time as coarsening. The time-resolved x-ray data obtained as a function of miscut further demonstrate that kinetic growth models based on adatom diffusion on singular surfaces are missing essential physical mechanisms which are step-edge density dependent.

$^1$Supported by the Cornell Center for Materials Research

4:18PM W20.00010 Nucleation of MB$_2$ thin films on Si by low temperature CVD: island statistics and growth kinetics. A. YANGUAS-GIL, N. KUMAR, J.R. ABELSON, Materials Science and Engineering Dep., U. of Illinois at Urbana-Champaign — HfB$_2$ thin films are deposited onto H-terminated Si by CVD using the single source precursor Hf(BH$_4$)$_2$, which affords extremely conformal and smooth film growth. HfB$_2$ films are technologically important as hard coatings and as impurity diffusion barriers. We analyze the nucleation process by in-situ spectroscopic ellipsometry (SE) and ex-situ AFM. The objective is to derive mechanistic information on the growth kinetics from a statistical analysis of the early stages of growth. The experimental results reveal that HfB$_2$ nucleates on Si(001) forming 3D islands and that there is an agreement between the SE data and the AFM measurements. Quantitative information on island statistics is extracted from AFM data taken after various growth times. The island height distribution functions are consistent with the presence of a physisorbed state of the precursor molecule. This situation is similar to that of the capture zone 2D island growth models in the literature and is in agreement with previous results on the steady state growth of HfB$_2$. The island spatial distribution and the correlation between island height and capture zone area indicate that nucleation is random and keeps on taking place until coalescence is reached. We show that the nucleation rate can be enhanced by surface activation, leading to a reduction in the grain size and lateral correlation length of the films.

4:30PM W20.00011 STM study of MOCVD-grown a-plane ZnO thin films: film thickness, growth temperature, and substrate miscut effects. O. DULUB, U. DIEBOLD, Department of Physics, Tulane University, New Orleans, Louisiana 70118, G. SARAF, Y. LU, Department of Electrical and Computer Engineering, Rutgers University, New Jersey 08854 — ZnO films with a-plane orientation were grown on r-plane (011bar2) sapphire substrates using metal-organic chemical vapor deposition (MOCVD). The surface morphology of ZnO films with various thicknesses (20 – 2000 nm), growth temperatures (300 - 580°C), and substrate miscut orientations and angles (0.2 - 2°) was characterized by low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Our results show strong dependence of surface morphology on growth parameters and the substrate miscut. STM images reveal uniform surfaces with small, rectangular terraces during the initial growth stage (20 nm-thick film). Films with thicknesses between 100 and 450 nm have a characteristic wave-like surface morphology with needle-shaped domains running predominantly along the crystallographic c-direction. Films with a thickness of 2000 nm exhibit more flat surfaces, but with c-oriented facets. We observed an increasing surface quality of the films with increasing growth temperature. Films grown at 580°C exhibit the flattest surface morphology. Film morphologies show strong dependence on the substrate miscut angle as well as on the miscut direction at all growth conditions.
region have weak net polar-orientations with H pointing towards the liquid. At high pH (pH ∼ 11), water species contributing to the different parts of the spectrum. The result shows that at low pH (pH < ∼ 2), water molecules in both ice-like and liquid-like composition of the oxides forming the scale, and in the residual stress levels are found.

**Wednesday, March 13, 2008 2:30PM - 5:18PM - Session W21 DCMP: Surfaces and Interfaces II** Morial Convention Center 213

2:30PM W21.00001 Nano-confined water on surfaces of metal oxide nanoparticles, ANDREY LEVCHENKO, JULIANA BOERIO-GOATES, BRIAN WOODFIELD, ALEXANDER KOLESNIKOV, NANCY ROSS, DAVID WESOLOWSKI, DAVID COLE, ALEXANDER KOLESNIKOV, UNIVERSITY OF CALIFORNIA — DAVIS TEAM, DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY, BRIGHAM YOUNG UNIVERSITY COLLABORATION, INTENSE PULSED NEUTRON SOURCE, ALEXANDRA NAVROTSKY, PETER A ROCK THERMOCHEMISTRY LABORATORY AND NEAT ORU, UNIVERSITY OF CALIFORNIA - DAVIS TEAM, YOICHIRO MATSUMOTO, The University of Tokyo — The thermal decomposition of ultrathin oxide layers on silicon surface was investigated with TPD technique. Oxide layers were formed on Si(100) at 400°C by exposure to O2 molecular beam. The desorption spectrum of SiO for the initial coverages between 1.7 and 2.6 monolayers exhibits a relatively low peak at the lower temperature and a high peak at the higher temperature. The former peak corresponds to the unstable binding state, where O atoms are presumably trapped at the dangling bonds. The latter corresponds to the more stable binding states of O atoms at the dimer bridge sites and the dimer backbone sites. The most of O atoms are at the stable binding states, from which the desorption rate is well described by Avrami kinetics. This result is consistent with the reaction model which takes account of the void formation and growth as observed in STM studies. The rate-determining step is the reaction at void perimeter even if the overlap between voids becomes quite large. The Avrami exponents determined from our experiment suggest that the increase in the initial coverage makes the oxide adlayer more stable and suppresses the rate of void nucleation at the potential nucleation sites.

2:42PM W21.00002 X-ray Reflectivity Study of Thermal Capillary Waves and the Interfacial Profiles of Water-Alcohol Mixtures, YOONNAM JEON, JAEGO SUNG, DOSEOK KIM, Department of Physics and Program of Integrated Biotechnology, Sogang University, Seoul, Korea, WEI BU, DAVID VAKNIN, Ames laboratory and Department of Physics and Astronomy, Iowa State University, USA — The liquid/vapor interfaces of water-alcohol (methanol, ethanol, and propanol) mixtures were investigated by X-ray reflectivity. Analysis of X-ray reflectivity data shows that the interfacial widths (surface roughnesses) of all mixtures at a fixed temperature depend solely on the surface tension of the mixture, and the intrinsic surface roughness is on the order of inter-atomic distances, and within error, independent of solution constituents. The implications of our results in the regard to the origin of the intrinsic roughness and the capillary wave-vector cutoffs applicable to X-ray scattering will be discussed.

2:54PM W21.00003 Viscoelasticity of Water in Sub-nanometer Gaps1, TAI-DE LI, ELISA RIEGO, School of Physics, Georgia Tech, SCHOOL OF PHYSICS, GEORGIA TECH TEAM — Direct and simultaneous measurements of the normal and lateral forces encountered by a nanosize spherical silicon tip approaching a solid surface in purified water were reported. For tip-surface distances, 0.03nm < d < 2nm, experiments and grand canonical molecular-dynamics simulations find oscillatory solvation forces for hydrophilic surfaces, mica and glass, and less pronounced oscillations for a hydrophobic surface, graphite. The simulations reveal layering of the confined water density and the development of hexagonal order in layers proximal to a quartz surfase. For subnanometer hydrophilic confinement, the lateral force measurements show orders of magnitude increase of the viscosity with respect to bulk water, agreeing with a simulated sharp decrease in the diffusion constant. No significant viscosity increase is observed for hydrophobic surfaces.

3:06PM W21.00004 ABSTRACT WITHDRAWN —

3:18PM W21.00005 Study of Hydrophobic Water Interfaces with Phase-sensitive Sum-frequency Vibrational Spectroscopy1, CHUANSHAN TIAN, Y. RON SHEN, UC Berkeley — Self-assembled monolayer of octade-cytrichlorosilane (OTS) on fused silica has been used extensively as a representative hydrophobic surface in study of water/hydrophobic interfaces. However, the interfacial water structure and how it changes upon solvated ions are not clear. We have carried out a study on OTS/water interface using the newly developed phase-sensitive sum-frequency vibrational spectroscopy (PS-SFVS). It allows measurement of both real and imaginary parts of the surface spectral response with the latter playing a role equivalent to absorption and emission coefficients and provides information on net polar-orientations of various interfacial water species contributing to the different parts of the spectrum. The result shows that at low pH (pH< ∼ 2), water molecules in both ice-like and liquid-like region have weak net polar-orientations with H pointing towards the liquid. At high pH (pH> ∼ 11), they are well aligned with H pointing to the solid substrate. It is due to that OTS/silica is negatively charged at high pH because of the adsorption of OH⁻ ions on methyl groups of OTS, so that the surface field will reorient part of the interfacial water molecules.

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1Supported by NSF

2This work was supported by NSF grant through WaterCAMPWS.
3:30PM W21.00006 Electronic Structure and adsorption of Pentacene on Cu and Ag (110). ABDELKADER KARA, Department of Physics, University of Central Florida, Orlando FL32816 — The adsorption of pentacene (C_{22}H_{14}) at coverages of one and 0.8 monolayer on Ag(110) and Cu(110) is studied using density functional theory. The unit cells for these systems are 6x2 and 7x2 for Ag(110) and Cu(110), respectively. The pentacene molecule adsorbs nearly flat (with a structural corrugation of about 0.6 Å) at a position 2.5 above the surface. On Ag(110), the adsorbed pentacene is even flatter (0.45 corrugation) and sits higher (about 2.8 Å) than the case of Cu. On Cu(110), most of the carbon atoms adsorb on top of Cu atoms, which is not the case on Ag(110). The resulting changes in the electronic states and the nature of the bonding will be discussed and comparison between the two systems will be presented.

3:42PM W21.00007 Plasmonic Coupling of a Gold Colloid and a Gold Film, ALBERT CHANG, FEI LE, FELICIA TAM, NAOMI HALAS, PETER NORDLANDER, KEVIN KELLY, Rice University — Engineering of plasmon resonances is important for a variety of applications, including but not limited to surface enhanced Raman spectroscopy (SERS) and near field scanning optical microscopy (NSOM). Of special interest are systems where the plasmons of a nanoparticle and a thin gold film are coupled. This coupling allows for a greater degree of control of the plasmon resonance of the system, as well as a strong, localized, enhancement of the incident electric field. We demonstrate that this coupling, and the resulting enhancement, can be used for SERS applications, and explore its impact on potential NSOM applications.

3:54PM W21.00008 Dipole interactions between dielectric spheres in AC electric fields, MANISH MITTAL, ERIC FURST, University of Delaware — Rheological properties of Electrorheological (ER) suspensions change dramatically on application of electric field. One of the key issues in the study of ER fluids is the nature and strength of the forces between suspended particles. Micron-sized dielectric spheres aggregate to form linear chains on the application of an AC electric field. The dipole-dipole attraction is the dominant force in this process. The dipole moment has contributions from Maxwell-Wagner charge distribution and the double layer polarization. Using optical tweezers the force between a pair of polystyrene spheres has been measured by observing the displacement of particle held in a static optical trap, of known trap stiffness, from its equilibrium position. At a fixed salt concentration, frequency and electric field strength the radial and tangential force have been measured as a function of the center-to-center separation (r) and angle (θ) with the electric field to create a 2-dimensional force map. Such a complete 2-dimensional interaction profile of micron-sized particles has never been measured before. Subsequently the effect of field, frequency and background salt concentration was studied. It was found that adding salt and increasing field frequency suppressed dipolar interactions. This effect can be explained qualitatively by the double layer polarization theory. Finally the effect of particle geometry was studied by measuring interactions between particles of different size and shape.

4:06PM W21.00009 Gap-mode enhanced Raman scattering of organic monolayers on flat Au(111) surface, KATSUYOSHI IKEDA, NORIHIRO FUJIMOTO, KOHEI OUSAKI, HOKKAIDO UNIVERSITY TEAM — A metal-molecule junction is recognized as a fundamental issue of molecular-based nano-devices. Charge transport through organic layers is strongly affected by chemical and physical properties of metal-molecular interfaces. In order to investigate molecular structures adsorbed on metal surfaces, surface-enhanced Raman scattering (SERS) is widely utilized as a powerful spectroscopic tool. Because of the electromagnetic origin of SERS, however, conventional SERS spectroscopy is applicable only for "rough" metal surfaces. Since various adsorption sites are exposed on rough metal surfaces, it is difficult to obtain intrinsic information of metal-molecular junctions. Here, we provide a simple method of enhanced Raman spectroscopy for organic monolayers on "flat" metal surfaces based on gap-mode plasmon excitation. The gap-mode enhanced Raman spectra measured on "flat" Au(111) single crystal facets were compared with conventional SERS spectra, and adsorption site dependence of molecular structures was discussed.

4:18PM W21.00010 Cooperative plasmon-mediated fluorescence of molecules near a metal nanoparticle, V. N. PUSTOVIT, T. V. SHAHBAZYAN, Jackson State University — We study radiative and nonradiative decays of an ensemble of molecules attached to a metal nanoparticle. We show that when the system size is smaller than the radiation wavelength, the excited molecular dipoles are hybridized with each other via the nanoparticle surface plasmon, leading to cooperative plasmon-mediated emission similar to Dicke superradiance. In particular, an ensemble of N molecules located at random positions but at the same distance from nanoparticle surface has only 3 bright (superradiant) eigenstates each characterized by the single-molecule plasmon-enhanced radiative decay rate multiplied by approximately N/3, while the remaining N-3 states are optically dark (subradiant). The fluorescence quenching by the nanoparticle exhibits a similar behavior, with bright states having single-molecule nonradiative decay rate multiplied by the same factor and dark states having much longer still finite non-radiative lifetime due to contribution of higher angular momenta. As a result, the radiation power of an ensemble is thrice that of a single molecule near a nanoparticle irrespective to total number of molecules. Calculations were performed for both perpendicular and parallel dipole orientations with respect to the nanoparticle surface.

4:30PM W21.00011 Anisotropic mass enhancement factors of Γ state on Be(0001) surface, TJEY CHIEN, University of Tennessee, KNOXVILLE, ÉMILE RIENKS, MARIA JENSEN, Institute for Storage Ring Facilities and Interdisciplinary Nanoscience Center (INANO), University of Aarhus, Denmark, ASIER EIGUREN, EUGENE CHULKOV, Donostia International Physics Center (DIPC), 20018 San Sebastian/Donostia, Spain, PHILIP HOFMANN, Institute for Storage Ring Facilities and Interdisciplinary Nanoscience Center (INANO), University of Aarhus, Denmark, WARD PLUMMER, University of Tennessee, Knoxville — It is controversial on the values of mass enhancement factors, λ, of Be(0001) Γ state. Three possible explanations are: (1) λ is anisotropic along the Fermi circle; (2) method-based difference for extracting λ; (3) failure of theoretical model for capturing EPC features. We demonstrate a systematically survey of λ along the Fermi circle of Be(0001) Γ state. By adopting different methods to extract λ, the possibility of method-based inconsistency was ruled out. The trend of the anisotropic λ is clear and is confirmed by theoretical calculations, though the values are inconsistent with experiment. With model data simulation, we are confident about the extracted λ while we have noisy data. The possible explanation is that the DFT-LDA calculation can not catch the features of EPC on Be(0001) Γ state correctly. This work is financially supported by National Science Foundation (grants NSF-DMR-0451163).
4:42PM W21.00012 Electron-phonon induced complex quasiparticles in the 1x1 H/W(110) surface.¹, ASIER EIGUREN, Donostia International Physics Center (DIPC). CLAUDIA AMBROSCH-DRAKL, Montan University Leoben — We show that the solution of the complex Dyson equation for the electron-phonon problem induces several quasiparticle states for a given wave vector. The Dyson equation is considered in the full complex plane and it is solved without considering the imaginary part of the self-energy as a small parameter. By a first principle application of the formalism to the 1x1 H covered W(110) surface, we show that some aspects of the surface band splitting [Rotenberg et. al., Phys. Rev. Lett. 84, 2925 (2000)] can be traced back to electron-phonon coupling, where we present the energy and lifetimes of each quasiparticle. Despite this breakdown of the single quasi-particle picture, it is remarkable that the spectral functions are very well Represented by the predicted multiple quasi-particles. From these results, we can deduce that some of the features that previously where prescribed in ARPES spectra as incoherent structure could eventually be re-interpreted as contributions from additional quasi-particle states. Our method could also help to understand similar phenomena observed in high Tc cuprates and various other surfaces.

¹This work was support by the Austrians Science Fund, project P16227 and the Fellows Gipuzkoa program of DIPC.

4:54PM W21.00013 Light-enhanced diffusion at the solid-liquid interface, SUNG CHUL BAE, JANET WONG, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois — Positively-charged rhodamine 6G molecules were allowed to adsorb onto quartz and mica surfaces and their translational and rotational diffusion was studied simultaneously by combined fluorescence correlation spectroscopy and time-correlated single photon counting. Surprisingly, the surface translational diffusion coefficient increased in direct proportion to the laser power used to excite these dye molecules. To elucidate the diffusion mechanism, we have investigated the excitation wavelength dependence, the spatial position dependence of diffusion coefficients, and the correlations between rotation and translation motion.

5:06PM W21.00014 Epitaxial Growth of Quinacridone Derivative on Ag(110), XIAOBO HE, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China & University of Tennessee, Knoxville, TN 37936, JINMING CAI, DONDXIA SHI, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China, WERNER A. HOFER, Department of Chemistry, The University of Liverpool, Liverpool L69 2BX, UK, E. WARD PLUUMER, Oak Ridge National Lab, Oak Ridge, TN 37831 and Univ of Tennessee, Knoxville, TN 37936, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China. — The growth behavior of quinacridone-derivative (QAC10C) molecules on Ag(110) surface is studied using low-energy scanning tunneling microscopy and low energy electron diffraction. At low coverage two distinct molecular orientations can be observed on silver terraces. At higher coverage up to 1 monolayer, depending on the growth temperature we observe two different structures on Ag(110) surface. At 100K the molecules organize in a complete monolayer on the surface, with a network-like structure. At 300K, the molecular orientation on the surface gives rise to row-like ordering, with a substantially higher molecular density. A theoretical analysis reveals that the structure of the molecular layer is controlled by the competition between molecular deposition rates and molecular diffusion along the surface.

Thursday, March 13, 2008 2:30PM - 5:18PM — Session W22 DMP DPOLY: Focus Session: Organic Photovoltaics and LEDs — Center 214

2:30PM W22.00001 Probing Photoconductivity in Phthalocyanines by Terahertz Spectroscopy, CHEN XIA, BRIAN KUBERA, VOLODIMYR DÜZHKO, HEFEI SHI, KENNETH SINGER, JIE SHAN, Department of Physics, Case Western Reserve University — Liquid crystals (LCs) are a relatively new class of photoconductors. Surprisingly high carrier mobilities have lately been reported in LCs. Although the high photogeneration order in these systems has been recognized to play an essential role in the high carrier mobilities, the mechanism of charge transport and carrier photogeneration are still not well understood. In this work, we investigate phthalocyanine (Pc) derivatives belonging to a family of discotic LCs as a model system. Optical pump/terahertz probe spectroscopy was employed to measure frequency dependence of the photocconductivity in Pc from 0.2 to 2.5THz. Photoconductivity appears within ~1ps (limited by time resolution of setup) after photoexcitation. It is followed by a fast decay of a few ps and a slow decay of 10's ps. Distinct frequency dependences were observed in the polycrystalline and liquid crystalline phases. The mechanism of charge transport and free carrier generation and recombination in the material will be discussed.

2:42PM W22.00002 Solution Processed Carbon Nanotube /PMMA Nano Composite Infrared Photodetectors, YI LIU, LIWEI LIU, PAUL STOKES, QUN HUO, SAIFULI KHONDAKER, University of Central Florida, NANOSCIENCE TECHNOLOGY CENTER, DEPARTMENTS OF PHYSICS & CHEMISTRY, UNIVERSITY OF CENTRAL FLORIDA TEAM — Solution processable nanostructured materials are of great interest for electronic and optical devices because of their enhance functionality, easy processibility, flexibility, and low cost of fabrication. We tested multi walled carbon nanotube networks dispersed in poly (methyl methacrylate) (PMMA) matrix for use as the infrared (IR) photodetectors at room temperature in ambient condition. Our study reveals both negative and positive infrared response depending upon the dark conduction of the composite. The temperature dependence of resistance, photo intensities and bias voltages dependence of IR response will be presented. This work shows promising novel route for the fabrication of infrared bolometric photo detector based on solution-processed carbon nanotube/PMMA composites.

2:54PM W22.00003 Triplet excitons in a ladder-type conjugated polymer: application in organic optoelectronics¹, K. YANG, M. ARIF, S. GUHA, University of Missouri-Columbia — Trace concentrations of metallic impurities present at the ppm level in conjugated polymers allow photophysical studies of triplet states at room temperature. We present temperature- dependent photoinduced absorption (PIA) and photoluminescence studies of diaryl (diphenyl)-substituted ladder-type poly (paraphenylene) (PhLPPP) containing a trace concentration of covalently bound Pd atoms. The T₁-T₂ peak (~1.3 eV) observed in the PIA blue shifts with increasing temperatures at a rate higher compared to the blue shift of singlet excitons in the sample with increasing temperatures. The temperature shift of the PIA signal arises both due to the temperature dependence of the triplet mobility as well as its mean free path. Our observations suggest that with increasing temperatures the triplet excitons remain localized on smaller chain segments. A triplet lifetime of ~12 ms was determined at room temperature. Furthermore, we will discuss the application of triplet state enhanced polymers in photovoltaic applications.

¹We thank Prof. U. Scherf for the donation of the material. This work was supported by NSF-ECCS # 0523656.
3:06PM W22.00004 Photovoltaic Effect in a Composite involving the Nonconjugated Conductive Polymer, Poly(β-pinene) and C_{60}, ADITYA KUMAR PALTII, ANANTHAKRISHNAN NARAYANAN, MRINAL THAKUR, Photonic Materials Research Laboratory, Auburn University, AL — Photovoltaic effect in a composite involving a nonconjugated conductive polymer, poly(β-pinene) and C_{60}, will be reported. The photovoltaic cell was fabricated using indium tin oxide coated glass as one electrode and aluminum as the other, with a poly(β-pinene)-C_{60} composite film sandwiched between the electrodes. Nitrogen laser (emission at 325 nm) and illuminant white light bulbs (emission at 300-700nm) were used as the light sources and the photo-voltage produced was recorded for different light intensities. The photo-voltage produced had a linear dependence on the light intensity. About 100 mV was generated for an intensity of ~4 mW/cm^2. Pristine poly(β-pinene) has a photoluminescence peak at 360 nm for excitation at 280 nm. As we have observed, this photoluminescence is quenched when C_{60} is added to poly(β-pinene) to form the composite. Therefore, the observed photovoltaic effect appears to be a result of excited-state electron transfer from poly(β-pinene) to C_{60}.

3:18PM W22.00005 Femtosecond and CW transient studies of photoinduced charge transfer in donor/acceptor blends for organic solar cells1, JOSH HOLT, SANJEEV SINGH, TOMER DRORI, ALEXANDRE NDOBE, Z. VALY VARDENY, University of Utah — Current developments in organic solar cells (~6% power conversion efficiency) require understanding and control of photoinduced charge transfer donor-acceptor pairs. In this work we provide and compare evidence that poly(2-methoxy-5(2′-ethyl)hexoxy-phenylenediyline) (MEH-PPV, donor) blended with 2,4,7-trinitrofluorenone (TNF, strong acceptor) form a below-gap charge transfer complex (CTC) state that extends absorption into the near infrared (NIR). Transient PA measurements show direct photoexcitation into the CTC state where significant charge species are initially photogenerated, the majority of which geminately recombine within ~10 ps, but the few that escape geminate recombination are subsequently captured in long-lived traps. Polaron could also be photoexcited with high efficiency at NIR excitation, with similar fate. This shows that a CTC state exists below the MEH-PPV optical gap, but with low dissociation efficiency, which leads to poor photovoltaic effect. We compare our results to those in blends of MEH-PPV/C_{60}, where apparently the obtained CTC state has a much higher dissociation efficiency.

1Supported in part by DOE grant No. 04-ER 46109.

3:30PM W22.00006 Quantum efficiency in organic phototransistors, WILLIAM HAMMOND, JIANGENG XUE, University of Florida — Organic optoelectronic devices hold a prominent role in current applied physics research. Although these devices inherently suffer from lower carrier mobility than inorganic devices, their mechanically flexible nature and low material costs enable new and interesting applications. Organic phototransistors, for example, may enable simplified circuits for large area and flexible sensors. Here we report the spectral dependence of the external quantum efficiency of organic phototransistors (OFETs) based on pentacene and C_{60}. Furthermore, we explore the gain mechanism in these devices and the effect of transistor structure on internal photomultiplication.

3:42PM W22.00007 Ultrafast dynamics in blends of π-conjugated polymers/fullerenes1, SANJEEV SINGH, MINGHONG TONG, CHUANXIANG SHENG, ZEEV VARDENY, University of Utah — We have studied the ultrafast dynamics of photogenerated charges and excitons in a variety of π-conjugated polymer/fullerene blends using the transient pump-probe photomodulation (PM) spectroscopy with ~100 fs resolution. These composites serve as active layers in organic photovoltaic devices with high power conversion quantum yield, due to the existence of a photoinduced charge transfer (PCT) reaction between the polymer and the fullerene molecules. Our transient PM spectrum spans a broad energy range from 0.1-2.4 eV, and this allows us to monitor the transient behavior of the various photoinduced absorption (PA) bands of polaron and excitons in the PM spectrum; as well as the transient excitation stimulated emission, and photoelectrochemical (PB) of the ground state. The PB dynamics reflect the ground state recovery; hence, it can be used to determine the long-lived polaron photogeneration quantum efficiency in these systems.

1Supported in part by the DOE grant 04-ER 46109 at the University of Utah.

3:54PM W22.00008 Spin Response in Organic Light Emitting Diodes1, FUJIAN WANG, CUNGENG YANG, TOMER DRORI, Z. VALY VARDENY, Department of Physics, University of Utah — To understand the origin of the magnetic field effect in OLEDs, we studied the large magnetoresistance (MR) and magneto-electroeluminescence (MEL) of OLEDs based on pristine MEH-PPV polymer, as well as MEH-PPV doped with various concentrations of radical impurities and C_{60} molecules. In contrast to OLED based on pristine MEH-PPV that show MR and MEL up to 12% at room temperature, we found in MEH-PPV:C_{60} based OLED the MR and MEL decrease substantially with increasing C_{60} molecule concentration. For MEH-PPV:C_{60} devices with C_{60}, concentration of 50%, the MR effect is less than 0.3% at room temperature. In MEH-PPV:radical devices the MR and MEL effects again differ substantially from those found in pristine and C_{60} doped MEH-PPV devices. At 50% radical concentration the MR and MEL effects are about 1% and 3.5%, respectively. The results are discussed with existing models for the magnetic field effects in OLEDs.

1Supported in part by the DOE and NSF DMR at the University of Utah.

4:06PM W22.00009 Organic Semiconductors: devices, growth and ordered assembly1, FABIO CICOIRA, Cornell University — Organic semiconductors are employed in devices such as field-effect transistors (FETs), light-emitting diodes and photovoltaic cells. Besides their technological interest, these devices are model systems to study physical processes in organic semiconductors [1]. Light-emitting field effect transistors (OLEFETs) based on organic semiconducting films are a novel class of devices integrating the transistor function with the light emission [2]. I will discuss LEFETs based on oligothiophenes [3] and oligoacenes [4][5], in particular their optoelectronic properties and the films growth physics. A unique property of organic semiconductors is the ability to form ordered assemblies at surfaces that can be studied by scanning tunneling microscopy (STM). I will discuss the growth and architectural motifs of copper of two organic semiconductors: the linear and planar quinqueithiophene [6] and the branched non-planar rubrene [7]. These studies show the ability of organic semiconductors to form fascinating self-assembled motifs and are of paramount importance to understand the early stages of growth of organic films. Organic electrochemical transistors (OECTs) are expected to play a key role in future organic electronics. OECTs are ideal candidates for biosensing applications thanks to their low driving voltage and their ability to operate in aqueous environment. A great deal of work is needed to understand the device physics of OECTs and optimize their performance. I will discuss advances in the field drawing examples from studies on devices based on the conducting polymer PEDOT:PSS.

1Support from the European Union under grant MOIF-CT2006-040864 is acknowledged.
Spin injection effects on exciton distributions in conjugated organic semiconductors, Mohammad Yunus, Paul Paul, Darryl Smith, and Lee Alamos National Laboratory — Conjugated organic semiconductors are under rapid development as the active material in organic light emitting diodes (OLEDs). Experiments and holes injected into the organic semiconductor form bound singlet or triplet excitons. Singlet excitons may recombine radiatively giving rise to light emission whereas triplet excitons do not recombine radiatively. Thus the quantum efficiency of OLEDs is limited by the fraction of singlet excitons, χS. In this work, we explore theoretically an approach to control χS through spin-polarized electron and hole injection from ferromagnetic contacts. Conventional ferromagnetic transition metals and half-metallic materials, such as LSMO, are considered as candidate electrode materials. The electron and hole transport in the organic semiconductor is treated through the conventional device equations with the formation of excitons described by a Landegev process. Once formed, the excitons may recombine or diffuse. Triplet excitons have a lower recombination probability and hence a longer diffusion length. The model calculations yield steady state spatial profiles for singlet and triplet exciton densities in the organic semiconductor.

This work was supported in part by NSF-ECS.

Electrically detected coherent spin manipulation of polaron pairs in an MEH-PPV OLED, Heather Seipel, Dane Mccamey, Seoyoung Paik, Manfred Walter, Nick Borys, John Lupton, Christoph Boehme, Department of Physics, University of Utah — Understanding of spin relaxation in organic light emitting diodes (OLEDs) is important for determining the maximum device efficiencies, due to the spin dependence of electronic transitions in organic materials. Here, we present an experiment demonstrating that coherent spin motion of polaron spin pairs can influence the current through an OLED fabricated using the prototypical conjugated polymer poly[2-methoxy-5-(2-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV). We observe a change in the zero-bias photocurrent transient through an OLED device following a short, coherent microwave pulse resonant with polaron pair spin transitions. The shape of the current transient provides information about the recombination rates of polaron pairs in both the singlet and triplet configurations. By varying the length of this pulse, coherent Rabi oscillations are detected, which reveal that the polaron pairs sensitive for the signal remain coherent for >0.5 µs. Due to these extremely long coherence times, we conclude that spin mixing processes are unable to significantly influence the spin state of the polaron pairs.

Tunable and White Light Emitting Diodes of Single Component Fluorinated Benzoxazole Graft Copolymers, Shih Jung Bai, Chienu-Chang Wu, Institute of Materials Science and Engineering, National Sun Yat-sen University — Coil-like graft copolymers of poly(Am-co-B-(1-x)) containing identical heterocyclic aromatic benzoxazole with trifluoromethyl-ethyl as the backbone and pendant of monohydroxyl (Am) and/or di-acyloxy (B-(1-x)) on their phenylene ring were studied for luminescence properties. The copolymers were synthesized with molar fraction m ranging from 0.25, 0.5, 0.75 to 1, and then dissolved and spun onto Spectrosol® quartz slide or indium-tin-oxide (ITO) substrate. The fluorescence and PL emissions of copolymers were investigated by ultraviolet-visible absorption covering 185 nm to 800 nm and photoluminescence (PL) emission excited at 363 nm. The PL results exhibited an excellent chromatic tuning range from green to white emission as m decreased. Aluminum electron injectors were evaporated onto the copolymer/ITO unit making it into mono-layer light emitting diodes for current-voltage and electroluminescence (EL) responses. An emission threshold voltage of 6 V was achieved for all the mono-layer copolymer devices. The Commission Internationale de l’Eclairage chromaticities of the EL emission were from (0.25, 0.53) to (0.24, 0.31) covering a wide visible range including white light emission.

Parameters controlling magnetic transitions in manganites, B. Dabrowski, S. Kolessnik, O. Chmaissem, J. Mais, Department of Physics, Northern Illinois University, DeKalb, IL 60115, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 — Using description of structural and physical properties of perovskites in terms of the tolerance factor t(x,T,d), which is dependent on composition, temperature, and oxygen-content, we have established synthetic methods and studied composition-structure-properties for new manganites La1−xSrxBaMnO3+δ. These are stable solid solutions limits normally achieved during the synthesis in air. Parameters controlling magnetic transitions have been identified through examples of single-valent compounds of RmO3 (the Mn-O-Mn bond angles that can be equivalently described in terms of the tolerance factor) and Sr1−xCa2MnO3 (the tolerance factor and the variance of A-site ion sizes), and the mixed-valent La0.5Sr0.5BaMnO3 (the tolerance factor, variance of sizes, and the local strains described in terms of the elongated Mn-O bonds). By using an example of kinetically stable, atomically-ordered layered-perovskites RSm2MnO6 we show that the increase of Curie temperature Tc and enhancement of colossal magneto-resistive effect at room temperature, can be achieved through reduction of variance of sizes and local strains. Work at NIU was supported by the NSF-DMR-0302617 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

Parameters controlling magnetic transitions in manganites, B. Dabrowski, S. Kolessnik, O. Chmaissem, J. Mais, Department of Physics, Northern Illinois University, DeKalb, IL 60115, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 — Using description of structural and physical properties of perovskites in terms of the tolerance factor t(x,T,d), which is dependent on composition, temperature, and oxygen-content, we have established synthetic methods and studied composition-structure-properties for new manganites La1−xSrxBaMnO3+δ. These are stable solid solutions limits normally achieved during the synthesis in air. Parameters controlling magnetic transitions have been identified through examples of single-valent compounds of RmO3 (the Mn-O-Mn bond angles that can be equivalently described in terms of the tolerance factor) and Sr1−xCa2MnO3 (the tolerance factor and the variance of A-site ion sizes), and the mixed-valent La0.5Sr0.5BaMnO3 (the tolerance factor, variance of sizes, and the local strains described in terms of the elongated Mn-O bonds). By using an example of kinetically stable, atomically-ordered layered-perovskites RSm2MnO6 we show that the increase of Curie temperature Tc and enhancement of colossal magneto-resistive effect at room temperature, can be achieved through reduction of variance of sizes and local strains. Work at NIU was supported by the NSF-DMR-0302617 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

Parameters controlling magnetic transitions in manganites, B. Dabrowski, S. Kolessnik, O. Chmaissem, J. Mais, Department of Physics, Northern Illinois University, DeKalb, IL 60115, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 — Using description of structural and physical properties of perovskites in terms of the tolerance factor t(x,T,d), which is dependent on composition, temperature, and oxygen-content, we have established synthetic methods and studied composition-structure-properties for new manganites La1−xSrxBaMnO3+δ. These are stable solid solutions limits normally achieved during the synthesis in air. Parameters controlling magnetic transitions have been identified through examples of single-valent compounds of RmO3 (the Mn-O-Mn bond angles that can be equivalently described in terms of the tolerance factor) and Sr1−xCa2MnO3 (the tolerance factor and the variance of A-site ion sizes), and the mixed-valent La0.5Sr0.5BaMnO3 (the tolerance factor, variance of sizes, and the local strains described in terms of the elongated Mn-O bonds). By using an example of kinetically stable, atomically-ordered layered-perovskites RSm2MnO6 we show that the increase of Curie temperature Tc and enhancement of colossal magneto-resistive effect at room temperature, can be achieved through reduction of variance of sizes and local strains. Work at NIU was supported by the NSF-DMR-0302617 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

Phase separation in (001) and (110) La2/3Ca1/3MnO3 epitaxial films, J. Fontcuberta, I.C. Infante, F. Sanchez, Institut de Ciencia de Materials de Barcelona-CSIC, Campus UAB, 08193 Bellaterra, Spain, M. Wojcik, E. Jedryka, Institute of Physics, Polish Acad. of Sci., Al. Lotnikow 32/46, 02668 Warszawa, Poland, S. Estrade, J. Arbiol, F. Peiro, EME/CerMAE/IN2UB, Universitat de Barcelona, 08028 Barcelona, Spain — Recent reports on the formation of a highly conducting layer at the interface between two insulators have driven a strong interest to interface physics. To explore strain and polarity effects on electronic phase separation (PS), we have grown epitaxial films of La2/3Ca1/3MnO3 (LCMO) on (001) and (110) SrTiO3 (STO) substrates. (001) LCMO/STO and (110) LCMO/STO interfaces differ on the polarity sequence. Measurements of the LCMO layers show that the (110) LCMO films display always “better” magnetic properties that their (001) LCMO counter-partners and do not show any traces of PS. Moreover, we have analyzed the properties of (001) and (110) thin LCMO films capped with a thin STO barrier and compared with those of bare LCMO films. It turns out that STO capping induces PS in (001) LCMO films but not in (110) films. Reasons for this asymmetrical behaviour will be discussed.

Crystal Properties of Oxygen Composition Controlled La1−xSrMnO3+δ Single Crystals, Yuji Yokota, Jun-Ichi Shimoyama, Tetsuro Ogata, Atsushi Nakamura, Hiraku Ogino, Shigeru Horii, Kohji Kishino, Department of Applied Chemistry, University of Tokyo Team — The La1−xSrMnO3+δ is known to have various magnetic and crystal structures as functions of x. Although this system has relatively large oxygen nonstoichiometry, the effects of excess oxygen on the crystal structure and physical properties have not been well understood. In the present study, the crystal structure and physical properties of excess oxygen controlled La1−xSrMnO3+δ single crystals were systematically studied. Single crystals with nominal compositions of La1−xSrMnO3+δ (0.05 ≤ x ≤ 0.2) were grown by the floating zone method. Thin plate-like crystals were obtained from the grown boules and controlled the oxygen content by post-annealing in various atmospheres. With increasing δ, the orthorhombic of the as-grown La0.95Sr0.05MnO3+δ crystal changed to the rhombohedral through pseudo-cubic orthorhombic. In addition, ferromagnetic behaviors appeared accompanying the CMR effect and Tc increased as a function of δ. These are attributable to an increase of valence of Mn by excess oxygen. Relationships among the Sr substitution level, excess oxygen content, crystal structure and magnetic behaviors of La1−xSrMnO3+δ will be discussed.
3:06PM W23.00004 Improved CMR properties of RE-doped (La,Sr)MnO$_3$ single crystals  JUN-ICHI SHIMOYAMA, Department of Applied Chemistry, University of Tokyo, TETSURO OGATA, YUUI YOKOTA, HIRAKU OGINO, SHIGERU HORII, KOHJI KISHIO — The relationships among crystal structure, $T_C$ and CMR effect have been eagerly studied for (La,Sr)MnO$_3$ system mainly as a functions of the Sr composition, x thus far. In the present study, we have attempted to improve the CMR properties near room temperature of the present system by optimizations of $T_C$ and $T_C$ phase transition temperature between orthorhombic and rhombohedral through RE mixing and elimination of excess oxygen, i.e. cation vacancies, for (La$_{1-x}$Sr$_x$)$_3$MnO$_7$ single crystals with $x = 0.2$ and 0.25, which have higher $T_C$ than room temperature and essentially high electronic conductivity. Crystal boules with nominal compositions of La$_{0.75-x}$Pr$_x$Sr$_{0.25}$MnO$_7$ ($x = 0.0, 0.05, 0.15$) were grown by the floating zone method. Crystal structure of La$_{0.75-x}$Pr$_x$Sr$_{0.25}$MnO$_7$ at $\sim 300$ K changed from orthorhombic ($z = 0, 0.15, 0.25$) to orthorhombic ($z = 0.3$) due to a decrease in mean ionic radius of A site. In addition, Pr-doping systematically decreased the coexistence at different length scales of ferromagnetic, charge/orbital order has been recently recognized as an intrinsic feature of several strongly correlated electron systems. Using inelastic neutron scattering, we have studied the spin dynamics of the archetypical material (La,Pr)$_3$Ca$_{3-x}$MnO$_7$, where competing ground states coexist at low temperature. The low-$T$ spin wave excitations at $H = 0$ and $2T$ are drastically different. We discuss this difference in terms of magnetic excitations from ferromagnetic clusters of different length scales.

3:18PM W23.00005 Unconventional spin-dynamics in a phase separate, weakly disordered perovskite manganite$^1$, FENG YE, JAIME FERNANDEZ-BACA, PENGCHENG DAI, HYE-JUNG KANG, JEFFREY LYNN, CHENGLIN ZHANG, S.-W. CHEONG — The intense investigation of perovskite manganites has revealed a variety of fascinating properties. The phenomena known as phase separation, the coexistence at different length scales of ferromagnetic, charge/orbital order has been recently recognized as an intrinsic feature of several strongly correlated systems. With a new analytic model and inelastic neutron scattering, we have studied the spin dynamics of the archetypical material (La,Pr)$_3$Ca$_{3-x}$MnO$_7$, where competing ground states coexist at low temperature. The low-$T$ spin wave excitations at $H = 0$ and $2T$ are drastically different. We discuss this difference in terms of magnetic excitations from ferromagnetic clusters of different length scales.

3:30PM W23.00006 Phase separation in Pr$_{0.55}$Ca$_{1.45}$MnO$_{3.1+}$ evidenced by magnetic excitations$^1$, SONGXUE CHI, The University of Tennessee, Knoxville, FENG YE, JAYMIE LAMOUR, University of Tennessee, Knoxville, FENG YE, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory, HYE JUNG KANG, JEFFREY W. LYNN, YING CHEN, NIST Center for Neutron Scattering, YOSHIO KANEKO, YOSHINORI TOKURA, University of Tokyo — At doping levels $x \approx 0.5$, a coexistence of commensurate (CM) and incommensurate (ICM) magnetic peaks are observed in single-layered manganites Pr$_{1-x}$Ca$_{1+x}$MnO$_3$ with elastic neutron scattering. Temperature dependence measurements of the magnetic intensities with different energy resolutions indicate a glassy nature of the magnetic moments. The magnetic excitation measurements using inelastic neutron scattering on the $x=0.45$ system reveal both symmetric and asymmetric behaviors about the CM peak positions. This strongly suggests two types of magnetic excitations originated from separated phases: the CE-type magnetic phase and an additional electronic phase caused by extra electrons introduced into the CE template.

3:42PM W23.00007 Signature of Magnetic Phase Separation in Pr$_{1-x}$Ca$_{x}$MnO$_3$,$^1$ DALGIS MESA, HAO SHA, JIANDI ZHANG, Florida International University, Miami, FL 33199, F. YE, Oak Ridge National Laboratory, Oak Ridge, TN 37831, P.C. DAI, J. A. FERNANDEZ-BACA, Oak Ridge National Laboratory, HYE JUNG KANG, JEFFREY W. LYNN, YING CHEN, NIST Center for Neutron Scattering, YOSHIO KANEKO, YOSHINORI TOKURA, University of Tokyo — At doping levels $x \approx 0.5$, a coexistence of commensurate (CM) and incommensurate (ICM) magnetic peaks are observed in single-layered manganites Pr$_{1-x}$Ca$_{1+x}$MnO$_3$ with elastic neutron scattering. Temperature dependence measurements of the magnetic intensities with different energy resolutions indicate a glassy nature of the magnetic moments. The magnetic excitation measurements using inelastic neutron scattering on the $x=0.45$ system reveal both symmetric and asymmetric behaviors about the CM peak positions. This strongly suggests two types of magnetic excitations originated from separated phases: the CE-type magnetic phase and an additional electronic phase caused by extra electrons introduced into the CE template.

3:54PM W23.00008 Anomalous Short Range Charge Ordering in La$_{1-x}$Ca$_x$MnO$_3$ , JING TAO, Brookhaven National Lab, S.J. PENNYCOOK, Oak Ridge National Lab, Y. ZHU, Brookhaven National Lab — Long range charge ordered (CO) phases have been observed at low temperatures in manganites in certain doping ranges. Structural characterization of the long-range CO phase showed that the CO superlattice is always along the $a$ axis in bulk samples [1]. Here we report the observations of a short range CO phase in La$_{1-x}$Ca$_x$MnO$_3$ samples as a function of cation concentration $x$, temperature and magnetic field using in-situ electron microscopy. We find short range CO nanoclusters with the CO superlattice in both perpendicular directions (a and c axes) in single crystal samples. The a and c axis nanoclusters have different densities, and show different dependences on temperature and magnetic field. Time evolution of the CO nanoclusters with the CO superstructure along the anomalous direction (c axis) is also recorded, which implies that the energy barrier between the two types of the CO structure is very small [2] [1]. P. G. Radaelli et al., PRB 59, 14440 (1999) [2]. Research sponsored by the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and by appointment to the ORNL Postdoctoral Research Program administered jointly by ORNL and ORISE. Work at BNL was supported by the U.S. DOE/BES under Contract No. DE-AC02-98CH10886.

4:06PM W23.00009 Spatially-Resolved X-Ray Microstructural Studies of Bulk Phase Separation in Manganites$^1$, J.D. BUDAI, Oak Ridge National Lab, D.D. SARMA, Ind. Inst. of Sci., W. LIU, ANL, J.Z. TISCHLER, B.C. LARSON, ORNL, G. SHENOY, ANL, D. TOPWAL, Ind. Inst. of Sci., S.-W. CHEONG, Rutgers Univ. — We have used spatially-resolved, 3D x-ray microdiffraction to study phase separation in two directionally-solidified, transition-metal oxide systems: (Y,Eu)MnO and (Lu,La)SbMnO. Both systems exhibit micron-scale coexistence of separate single-crystal lamellar domains (hex/ortho and hex/thomb respectively) when grown by a floating zone method. Micron-resolution 3D x-ray microscopy reveals the domain morphologies, lattice orientations, and local strain fields within the phase-separated eutectic systems. The orientations of the lamellae are consistent with energetic predictions and the formation of low-energy, semi-coherent interfaces. In addition, we observe a bias for larger strain fluctuations in one phase. More generally, the microstructural features observed experimentally in these well-defined, micron-scale eutectic domains provide clues to the domain interactions believed to exist in similar, more homogeneous, nanoscale manganite systems. Structural studies at the nanoscale will be enabled in the future by advances in x-ray focusing optics.

1Supported by U.S. DOE under Contract No. DE-AC05-00OR22725 with UT/Battelle LLC.
2Supported by DOE-FG02-04ER46202. ORNL is managed by UT-Battelle, LLC for the U.S. Dept. of Energy under contract DE-AC05-00OR22725. This was also performed under the US-Japan Cooperative Program on Neutron Scattering.
3Supported by DOE DE-FG02-04ER46125. NSF DMR-0346826 and DMR-0453804.
4:30PM W23.00011 Domain Mapping of a Ca-doped Manganese, JOSHUA TURNER, University of Oregon, K. JESSICA THOMAS, MARY UPTON, JOHN HILL, Brookhaven National Laboratory, JEAN JORDAN-SWEET, National Synchrotron Light Source, YOSHINORI TOKURA, YASUHIDE TOMIOKA, Correlated Electron Research Center, STEPHEN KEVAN, University of Oregon — In the last few years, disorder has emerged as a key without which the colossal magnetoresistance (CMR) effect would not exist. Single crystals represent the simplest arenas to observe and study the peculiarities central to the manganites. This is in contrast to polycrystalline compositions for instance, where rampant strain fields can veil fundamental physics. By micro-focusing x-rays through a glass capillary, we have performed a microtopography technique to map the crystallographic domain structure of the Ca-doped manganese crystal, PCMO. This technique serves as a domain-mapping alternative tool to TEM that does not require challenging sample preparation procedures. Surprisingly, we find micron size domain structure. We suggest that the separation of crystallographic domains by twin boundaries is more relevant than previously believed. These boundaries could affect the large-scale, submicron size disorder that has been observed recently, and also may play a role in the heterogeneous nature of the CMR effect.

4:42PM W23.00012 Temperature-Dependent Electronic Structure of the Colossal Magnetoresistive Manganese La$_{0.7}$Sr$_{0.3}$MnO$_3$ via Hard X-Ray Photoemission, FRANCESCO OFFI, CNISM and Dip. di Fisica, Università Roma Tre, Rome, NORMAN MANNELLA, Physics, U. Tennessee Knoxville, GIANCARLO PANACCIONE, TASC-INFN-CNR, Trieste, Italy, TOMMASO PARDINI, Physics UC Davis, ANDREA FONDACARO, ESRF, Grenoble, PIERO TORELLI, CNR-INFN-S3, Modena, SIMO HUOTARI, ESRF, Grenoble, MARK WEST, Mat. Sci. Div., LBNL, JOHN MANN, Department of Physics and Astronomy, California State University, Los Angeles — We report magnetic susceptibility $\chi(T)$ measurements on oxygen-isotope exchanged La$_{1-x}$Ca$_x$MnO$_3$ up to 700 K. The $1/\chi(T)$ data show that the ferromagnetic exchange-energy $J$ depends strongly on the oxygen-isotope mass. The isotope effect on $J$ decreases with temperature up to 400 K and then increases again with temperature above 400 K. This unusual temperature dependence cannot be explained by existing theories of the colossal magnetoresistance effect for doped manganites. We suggest that a correct model for description of the physics of manganites should be based on double-exchange and the formation of localized bipolarons in the paramagnetic state.

5:06PM W23.00014 Origin of the Non-Linear Pressure Effects in Perovskite Manganites, ZHIQIANG CHEN, TREVOR TYSON, KEN AHN, New Jersey Institute of Technology, ZHONG ZHONG, Brookhaven National Laboratory, JINZHU HU, University of Chicago — High pressure resistivity and x-ray diffraction measurements were conducted on La$_{0.5}$Pr$_{0.5}$MnO$_3$ to $\sim$6 GPa and $\sim$7 GPa, respectively. At low pressures the metal-insulator transition temperature ($T_{MI}$) increases linearly up to a critical pressure, P* $\sim$ 3.4 GPa, followed by reduction of $T_{MI}$ at higher pressure. Analysis of the bond distances and bond angles reveal that a bandwidth increase drives the increase of $T_{MI}$ below P*. The reduction of $T_{MI}$ at higher pressures is found to result from Jahn-Teller distortions of the MnO$_6$octahedra. The role of anharmonic interatomic potentials is discussed.

5:18PM W23.00015 Phonon-induced magnetic deflagration and detection of very fast CMR in manganites, FERRAN MACIA, JOAN MANEL HERNANDEZ, GUILLER ABRIL, ALBERTO HERNANDEZ-MINGUEZ, Universitat de Barcelona, FRANCISCO PARISI, Comision Nacional de Energia Atomica, PAULO V. SANTOS, Paul-Drude Institut fur Korperelektronik, JAVIER TEJADA, Universitat de Barcelona — In this work we describe experiments in which we have used surface acoustic waves to induce controlled magnetic avalanches in (La, Pr)-based manganites. The avalanches propagate inside the sample following the law of the magnetic deflagration, and occur at well determined values of the temperature and the applied magnetic field, that depend on the phase separation fraction. Another important point is that the magnetic avalanche is accompanied by colossal variation of the electrical resistance in about 0.1 ms. F. Macia et al., Phys. Rev. B 76, 174424 (2007). F. Macia et al., Phys. Rev. B, submitted.

Surprisingly, thermally enhanced. For 260–302 K the onset time for photo-crystallization decreases with increasing temperature, but the crystallization rate is T-independent.

K. TANIOKA, NHK Laboratories, Tokyo — Photo-crystallization of amorphous (a-) Se is investigated as a function of temperature (T = 250–340 K) and exposure to 435 nm light. Raman scattering and modulated DSC on bulk As\(_2\)Se\(_3\) glasses result in the following observations: (1) the glass transition temperature (T\(_g\)) is 324 ± 2°C. (2) The rate of crystallization is 


Evidence for Quasi Tetrahedral S=As(S\(_1\)/\(_2\))\(_3\) local structures in As\(_x\)S\(_{1-x}\) glasses, PING CHEN, P. BOOLCHAND, C. HOLBROOK, Univ. Cincinnati, K. JACKSON, Central Mich., D. GEORGIEV, Univ. of Toledo, M. MICOLAULT, Univ. Paris — Raman scattering and modulated DSC on bulk As\(_x\)S\(_{1-x}\) glasses in the 0.08 < x < 0.41 range is studied\(^1\). We have examined a set of 4 samples (1181°C, 203°C, 324.7°C, 4254°C) with different T\(_g\)s indicated in parenthesis, in m-DSC, Raman and IR experiments to elucidate the role of bonded water. Our results show that the glass transition endotherm of sample 4 (dry) is characteristic of a stressed-rigid glass, while that of sample 1 (wet) of a flexible glass. Although Raman scattering of samples 1 and 4 look superficially similar, they are different in details; the Boson peak in sample 4 has a stronger intensity than in sample 1. IR reflectance function strength in the mid-IR range is weaker for sample 4 than for sample 1, and furthermore differs in details. These results show that presence of water disrupts the P-O-P chain network by replacing bridging O with terminal OH\(^-\) ends. And once water is bonded, it is difficult to remove it completely. These results will be compared to previous reports in the field. \(^1\) D.I. Novita and P. Boolchand Phys. Rev. B (in press) Supported by NSF grant DMR 04-56472.

Evidence of Intermediate Phase in (Na\(_2\)O)\(_x\) (GeSe\(_2\))\(_{1-x}\) glasses, V. ROMICHEVARLA, PING CHEN, D. NOVITA, P. BOOLCHAND, Univ. Cincinnati, M. MICOLAULT, Univ. of Paris, W. HUFF, Univ. Cincinnati — Intermediate phases have been observed in covalent glasses, but ionically bonded network systems have received much less attention in this respect. We have now examined titled glasses in m-DSC, Raman scattering, IR reflectance and Birefringence experiments over wide range of soda concentration, 3 < x < 30%. Thermal experiments reveal a sharp reversibility window (RW) in the 14% < x < 19% soda range, which correlates well with a broad global maximum in molar densities (germanate anomaly). Raman and IR reflectance TO and LO mode frequencies exhibit anomalies between x\(_1\) (1) = 14% (stress transition) and x\(_2\) (2) = 19% (rigidity transition), with optical elasticity power-laws confirming the nature of the transitions. Birefringence measurements dramatize the macroscopically stress-free nature of the Intermediate Phase (IP) in the RW. These data also suggest that the germanate anomaly can be understood as a direct consequence of the multiscale structural self-organization of glasses in the IP. \(^1\) Supported by NSF grant DMR 04-56472.

Competing effects in the photo-crystallization of a-Se HARP films, R.E. TALLMAN, B.A. WEINSTEIN, Physics Dept., SUNY at Buffalo, A. REZNIK, J.A. ROWLANDS, Sunnybrook Health Sciences Centre, Toronto. M. KUBOTA, K. TANIOKA, NHK Laboratories, Tokyo — Photo-crystallization of amorphous (a-) Se is investigated as a function of temperature (T = 250–340 K) and exposure time by Raman scattering in photo-active films used in high-gain avalanche rushing photoconductor (HARP) cameras. We observe different temperature regimes that reflect the competition of viscosity-driven and strain-driven processes. No photo-crystallization is seen below 260K, and above 318K the crystallization rate is thermally enhanced. For 260–302 K the onset time for photo-crystallization decreases with increasing temperature, but the crystallization rate is T-independent. Surprisingly, photo-crystallization is strongly suppressed in a 15 degree range around the glass transition at \(T_g\) ~ 310K. Our results are in qualitative accord with a theory by Stephens\(^1\) that treats the effects of local strain on the growth of crystalline-Se domains within an a-Se matrix – the strain arising from the density difference between the crystalline and amorphous phases. \(^1\) R.B. Stephens, J. Appl. Phys. 51, 6197 (1981).
2:30PM W25.00001 Design of Responsive Peptide-based Hydrogels as Therapeutics. JOEL SCHNEIDER, University of Delaware — Hydrogels composed of self-assembled peptides have been designed to allow minimally invasive delivery of cells in vivo. These peptides undergo sol-gel phase transitions in response to biological media enabling the three-dimensional encapsulation of cells. Peptides are designed such that when dissolved in aqueous solution, exist in an ensemble of random coil conformations rendering them fully soluble. The addition of an exogenous stimulus results in peptide folding into beta-hairpin conformation. This folded structure undergoes rapid self-assembly into a highly crosslinked hydrogel network whose nanostructure is defined and controllable. This mechanism, which links intramolecular peptide folding to self-assembly, allows temporally resolved material formation. In general, peptides can be designed to fold and assemble affording hydrogel in response to changes in pH or ionic strength, the addition of heat or even light. In addition to these stimuli, DMEM cell culture media is able to initiate folding and consequent self-assembly. DMEM-induced gels are cytocompatible towards NIH 3T3 murine fibroblasts, mesenchymal stem cells, hepatocytes, osteoblasts and chondrocytes. As an added bonus, many of these hydrogels possess broad spectrum antibacterial activity suggesting that adventitious bacterial infections that may occur during surgical manipulations and after implantation can be greatly reduced. Lastly, when hydrogelation is triggered in the presence of cells, gels become impregnated and can serve as a delivery vehicle. A unique characteristic of these gels is that when an appropriate shear stress is applied, the gel will shear-thin, becoming an injectable low viscosity gel. However, after the application of shear has stopped, the material quickly self-heals producing a gel with mechanical rigidity nearly identical to the original hydrogel. This attribute allows cell-impregnated gels to be delivered to target tissues via syringe where they quickly recover complementing the shape of the tissue defect. This shear-thin delivery method is a convenient way to introduce cells to wound sites.

3:06PM W25.00002 Synchrotron x-ray diffraction study on the size distribution and mechanical stability of microtubules by microtubule-associated-protein (MAP) tau, M.C. CHOI, U. RAVIV, H. MILLER, M. GAYLORD, E. KIRIS, D. VENTIMIGLIA, L. WILSON, M.W. KIM, S. FEINSTEIN, C.R. FAFNYA, UNIV. OF CALIFORNIA AT SANTA BARBARA TEAM, KOREA ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY TEAM, HEBREW UNIV OF JERUSALEM TEAM — In neurons, microtubules (Mts), 25nm protein nanotubes, are used extensively as tracks for transporting nutrients and cellular components between the cell body and axons. MAP tau regulates microtubule assembly and, in a poorly understood manner, inter-MT interactions. Altered tau-MT interactions leads to MT depolymerization and tau tangles, which is implicated in a large number of neurodegenerative diseases. We will show that the size distribution and the enhanced mechanical stability of Mts by tau bindings are dependent on tau isoforms. Supported by DOE DE-FG02-06ER46314, NSF DMR-053347, and NIH GM-59288, NIH RO1-NS35010.

3:18PM W25.00003 Effect of Mg Ions on Microrheological Properties of F-actin Solution across Isotropic-Nematic Phase Transition1, JUN HE, MICHAEL MAK, YIFENG LIU, JAY TANG, Brown University — We studied microrheological properties of F-actin across the isotropic-nematic phase transition region by video particle tracking and laser deflection particle tracking methods. The two methods give consistent results. As the nematic order parameter increases with the actin concentration, G’ (along the alignment) and G’’ grow apart, with G’’ larger than G’. The moduli scale with actin concentration as G’_c \propto \epsilon^{-0.542+0.13} and G’’_c \propto \epsilon^{1.38+0.15}. Furthermore, G’ and G’’ dependence on [Mg^{2+}] were measured and compared for 1 mg/ml isotropic and 4 mg/ml nematic F-actin solutions. For isotropic phase, G’ increase with [Mg^{2+}] up to 6 mM and then plateaus; for nematic phase, G’_c is larger and both G’ and G’’ increase with [Mg^{2+}] monotonically all the way up to 16 mM, above which F-actin bundle formation occurs. In both isotropic and nematic phases, G’’ only weakly depends on [Mg^{2+}]. In conclusion, particle tracking microrheology reveals rich rheological features of F-actin affected by I-N phase transition and by tuning weak electrostatic interactions among the filaments.

3:30PM W25.00004 The stability of cellulose, TONGYE SHEN, S. GNANAKARAN, T-Division, LANL — Stabilities and dynamics of cellulose, which is a common structural component of plants and microorganisms, are critical to understanding the biocompatibility and applications of cellulose-based materials. We studied the self-assembly of cellulose molecules by developing a computational model that accurately predicts the equilibrium properties of cellulose nanofibril assemblies. Our model reveals that hydrogen bonding (HB) stabilizes the nanofibril structure through a combination of intramolecular and intermolecular interactions. This understanding can guide the design of novel cellulose-based materials with improved properties for applications such as textiles and drug delivery.

3:42PM W25.00005 ABSTRACT WITHDRAWN —

3:54PM W25.00006 Transient Binding and Viscous Dissipation in Semi-flexible Polymer Networks, OLIVER LIELEG, TU Muenchen, Germany, MIREILLES CLAESSENS, Universiteit Twente, The Netherlands, ANDREAS BAUSCH, TU Muenchen, Germany — Nature specifically chooses from a myriad of actin binding proteins (ABPs) to tailor the cytoskeletal microstructure. Herein, cells rely on the dynamics of the cytoskeleton as its structural and mechanical adaptability is crucial to allow for dynamic processes. A molecular understanding of such biological complexity calls for an in vitro system with well-defined structural rearrangements and cross-linker dynamics to elucidate the physical origin of the unique viscoelastic properties of cells. As we present here, the frequency-dependent viscoelastic response of cross-linked in vitro actin networks is determined by the binding kinetics of cross-linking molecules. Independent from the particular network structure, the viscous dissipation (loss modulus) exhibits a pronounced minimum in an intermediate frequency which is dominated by elasticity. We show that in this frequency regime the molecular origin of the viscoelastic response is given by the non-static nature of actin/ABP bonds as they are subjugated to chemical on/off kinetics. The time scale of the resulting stress release is set by the lifetime distribution of the cross-linking molecule and therefore can be tuned independently from other relaxation mechanisms. We speculate that unbinding of distinct cross-links might be the molecular mechanism employed by cells for mechanosensing.

4:06PM W25.00007: Microtubule Self-Assembly, YONGSEOK JHO, M.C. CHOI, UCSB/KAIST, O. FARAGO, BGU, MAHNWON KIM, P.A. PINKUS, UCSB/KAIST — Microtubules are important structural elements for neurons. Microtubules are cylindrical pipes that self-assemble from tubulin dimers. We investigate the nature of the interactions which are essential to stabilize such the cylindrical assembly of protofilaments. We use Monte Carlo simulations to suggest the pathways for assembly and disassembly of the microtubules.

1Supported by NSF (DMR0405156) and PRF (42835-AC7).
5:06PM W25.00012 Dimensional percolation of sheared nano-rod dispersions and consequences for highly anisotropic property tensors1. M. GREGORY FOREST, University of North Carolina at Chapel Hill, XIAOYU ZHENG, Kent State University, RUHAI ZHOU, Old Dominion University, RICHARD VAIA, Nanostructured and Biological Materials Branch, AFRL/MLBP — The Doi-Hess theory for flowing nano-rod dispersion yields orientational probability distribution functions for the nano-particle phase in flow-processed thin films. These numerical databases for variable shear rate, particle aspect ratio and volume fraction are then combined with a Monte Carlo algorithm to populate sheared dispersions. Nano-rod cluster statistics are then computed to determine percolation thresholds, which yield transitions from zero to one, two and three dimensional percolating paths. Finally, effective property enhancements are computed which include standard volume-averaged homogenization and percolation cluster statistics.

1Research support from AFOSR FA9550-06-1-0063, NSF DMS-0604891

5:18PM W25.00013 Polymer Crystallization-Driven Gelation of an Ionic Liquid. DAVID HOAGLAND, JOHN HARNER, Univ. of Massachusetts Amherst — Polyelectrolyte gels and gels derived from polyelectrolyte solutions are a broad class of materials with diverse applications ranging from gelling agents in foods and pharmaceuticals to hydrogels in tissue engineering involving biomimetic self-assembly. We consider a class of ionic liquids that forms stable gel networks under the influence of physicochemical processing. 1-Ethyl-3-methylimidazolium ethyl sulfate [EMIM][EtSO4] is hygroscopic, and with water uptake, the modulus drops.

5:30PM W25.00014 Avalanches, hardening and softening in dense cross-linked actin networks. JAN ASTROM, CSC – Finnish IT Center for Science, Esbo, Finland, SUNIL KUMAR, Indian Institute of Technology Madras, India, ILPO VATTULAINEN, Tampere University of Technology, Finland, MIKKO KARTTUNEN, The University of Western Ontario, Canada — Actin filament networks enable cell motility, cell division and cell differentiation, and provide the framework for mechanical tension in animal cells. Actin filament networks can be thought of as flows of biopolymers through a random network of obstacles.

4:42PM W25.00010 Equilibrium Size Distribution of Twisted Biopolymer Bundles. GREGORY GRASON, University of Massachusetts, Amherst, ROBJIN BRUINSMA, University of California at Los Angeles — Using a continuum elastic model of hexagonal filament packing, we demonstrate that molecular-scale chirality strongly affects the equilibrium properties of aggregates, or bundles, of biopolymers, such as DNA and F-actin. We show that biopolymers tend to form bundles with long-range, chiral stress patterns, twisting or braiding helically around the central bundle axis. Due to the build-up of elastic stress on the outer surface, the cohesive energy of chiral filament bundles has a non-monotonic dependence on filament number. As a consequence, we demonstrate for two cases—bundles with 1) columnar-hexagonal order and 2) columnar-solid order—that a stable phase of dispersed bundles is thermodynamically stable below the point of bulk condensation and below a critical surface energy for the bundle exterior. This work suggests that the large characteristic radius biopolymer bundles observed in in vitro studies of is not a product of some mysterious long-range force or kinetic limitations of bundle growth, but rather in-plane elastic stresses which result from the local preference for the chiral packing of filaments.

4:54PM W25.00011 The Dependence of Actin Filament Assembly on Linking Agent Concentration. LAM NGUYEN, QI WANG, WEI YANG, LINDA HIRST, Florida State University — This experimental and computational study focused on the properties of actin filament bundles and networks induced by the actin filament cross-linker, α-actinin. Structural properties of actin filament networks linked by the α-actinin protein were studied experimentally by using confocal microscopy. We varied the concentrations of actin and linking agents to study their effects on the properties of the bundles and networks. The study showed that the molar ratio of α-actinin to actin played an important role in the properties of the network structure, determining the branching frequency of the bundles. An experimentally guided simulation based on the α-actinin/actin filament system was carried out using CHARMM to attempt to replicate the features of the real system and therefore to study the physics behind the actin filament assembly process in different regimes.

4:30PM W25.00009 Loop Closure Dynamics of Flexible and Semi-flexible Polymer. JEN-FANG CHANG, YENG-LONG CHEN, Academia Sinica, INST. OF PHYS., ACADEMIA SINICA TEAM, RCAS, ACADEMIA SINICA TEAM — It is widely believed that DNA looping due to multi-site DNA-binding proteins is important for DNA transcription, replication, and recombination. The chain closure problem has been studied in several Monte Carlo simulations to determine the chain closure probabilities and the chain conformation to infer dynamic properties. In this work, we investigate how the loop closure dynamics of flexible and semi-flexible polymers depend on the polymer length and the reactive site position using Brownian dynamics simulation, accounting for hydrodynamic interactions. Our study examines the probability of closing for two reactive sites along the chain and the shape of the loop formed by closing. In addition, intrachain hydrodynamic interactions are found to affect the diffusivity of circular chains compared to linear chains, in accord with experimental observations. We also consider the dynamics of chain closing under strong slt-like confinement as a function of slt height.

4:18PM W25.00008 Direct Observation of Early-Time Hydrogelation in β-Hairpin Peptide Self-Assembly. TUNA YUCEL, Materials Science and Engineering, University of Delaware, Newark, DE 19716, JOEL SCHNEIDER, Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, DARRIN POCHAN, Materials Science and Engineering, University of Delaware, Newark, DE 19716 — Triggered hydrogelation of MAX 1 peptide (NH2-(VK)17-PPT-(KV)17-CONH2) proceeds through peptide intramolecular folding into β-hairpins and immediate self-assembly into branched clusters of well defined (uniform, 3 nm cross section), semi-flexible, β-sheet-rich nanofibers. Cryogenic transmission electron microscopy indicates that dangling fibrils extend from one growing cluster to another and lead to early, intercluster communication in solution. At the apparent percolation threshold, the dynamic shear modulus measured by oscillatory rheology ($G'\omega$, $G''\omega$) and the field-intensity autocorrelation function measured by dynamic light scattering ($g_1(\tau) \times \tau^{-1}$) show power-law behavior with comparable critical dynamic exponents ($\nu \approx 0.47$ and $\beta \approx 0.45$). Finite interpenetration of percolating cluster with smaller clusters, along with permanent intercluster entanglements, increase the network rigidity. The self-assembly of MAX 1 peptide was contrasted and compared with the assembly of other biopolymeric networks in literature.
5:42PM W25.00015 Crystal aggregation in kidney stones; a polymer aggregation problem. J. WESSON, A. BESHENSKY, P. VISWANATHAN, W. ZACHOWICZ, J. KLEINMAN, Medical College of Wisconsin — Kidney stones most frequently form as aggregates of calcium oxalate monohydrate (COM) crystals with organic layers between them, and the organic layers contain principally proteins. The pathway leading to the formation of these crystal aggregates in affected people has not been identified, but stone forming patients are thought to have a defect in the structure or distribution of urinary proteins, which normally protect against stone formation. We have developed two polyelectrolyte models that will induce COM crystal aggregation in vitro, and both are consistent with possible urinary protein compositions. The first model was based on mixing polyanionic and polycationic proteins, in portions such that the combined protein charge is near zero. The second model was based on reducing the charge density on partially charged polyanionic proteins, specifically Tamm-Horsfall protein, the second most abundant protein in urine. Both models demonstrated polymer phase separation at solution conditions where COM crystal aggregation was observed. Correlation with data from other bulk crystallization measurements suggest that the anionic side chains form critical binding interactions with COM surfaces that are necessary along with the phase separation process to induce COM crystal aggregation.

Thursday, March 13, 2008 2:30PM - 5:18PM – Session W26 DCP: Focus Session: Advances in Atmospheric Aerosol Science IV Morial Convention Center 218

2:30PM W26.00001 "The optics of atmospheric aerosol particles". CHRISTOPHER SORENSEN, Kansas State University — No abstract available.

3:06PM W26.00002 The Molecular Picture Behind Resonance Phenomena in Aerosol Spectra. RUTH SIGNORELL, University of British Columbia, Chemistry Department — The study of icy aerosol particles with sizes in the submicron range is a highly interdisciplinary subject at the juncture of nanosciences, atmospheric physics, and astrophysics. The microphysics of aerosol clouds in the atmospheres of planets and their moons, such as ammonia clouds on Jupiter and Saturn or methane aerosols on Titan, is currently very much in the focus of the scientific community. Particularly broad interest has been sparked by the recent Cassini-Huygens mission to Saturn’s moon Titan, which has illuminated the importance of methane clouds for Titan’s weather and their analogy to the role of water ice clouds in Earth’s atmosphere. The present contribution focuses on the influence of intrinsic particle properties, such as shape, size or architecture, on infrared optical properties of icy aerosol particles. Intrinsic particle properties manifest themselves in mid-infrared extinction spectra by modifying the structure of vibrational bands. We ultimately aim at unravelling the microscopic origin of the characteristic patterns found in the spectra of these weakly bound molecular aggregates. To this end we compare our experimental results with different model calculations combining molecular dynamics simulations with vibrational quantum dynamics.

3:42PM W26.00003 Investigations of Hygroscopic Growth and Phase Transitions of Atmospheric Particles by Noncontact Atomic Force Microscopy (AFM). BENJAMIN OCKO, Brookhaven National Laboratory, SUSAN OATIS, University of New York, Stony Brook, MATTHEW STRASBERG, STEPHEN SCHWARTZ, ANTONIO CHECCO, Brookhaven National Laboratory — Aerosol particles (nanometer to micrometer sized particles suspended in air) affect atmospheric radiation and cloud microphysics. A correct description of their behavior in the atmosphere is essential to accurate climate modeling. The processes by which initially hydrophobic particles become hygroscopic, accrete water from the vapor, undergo phase transition from solid particles to solution droplets are important but not well understood at a fundamental level. We have carried out AFM studies to measure changes in particle size and morphology as a function of the relative humidity for particles of sodium chloride (a substance whose bulk hygroscopic properties are well characterized) deposited on substrates with differing surface energies (Silicon Oxide, Carboxy- and Methyl-terminated organic thin-films). For particles with height > 50 nm, deliquescence was observed with a relative humidity near 75% (±2%), is consistent with measurements of suspended aerosols. These preliminary results demonstrate that environmental AFM is a viable probe for studying the hygroscopic behavior of salt nanoparticles on solid supports. Supported by the U.S. Department of Energy, DE-AC02-98CH.

3:54PM W26.00004 Extinction by Single and Multiple Particles1. MATTHEW BERG, CHRISTOPHER SORENSEN, AMIT CHAKRABARTI, Kansas State University — The combined effect of scattering and absorption is referred to as extinction and is responsible for the redistribution of radiant energy by a particle. This presentation will show that extinction is due to wave interference. Simulations of the energy flow caused by the interference graphically demonstrate how extinction redistributes the energy of incident light. Both single and multi-particle systems are considered. A conceptual, phase-based explanation is given that builds on previous work and illustrates the physical meaning of the optical theorem. Implications regarding the measurement of extinction are discussed.

1Funded by the NASA Graduate Student Researchers Program

4:06PM W26.00005 Scattering Patterns for Spherical and Non-spherical Particles. CHRISTOPHER SORENSEN, Kansas State University — Aerosols affect our climate directly by scattering and absorbing light. These optical properties depend on the size, shape, and composition. We have recently described patterns that appear in the phase function for spherical particles. Mie scattering, when the scattered intensity is plotted versus the scattering wave vector q = 2ksin(theta/2) [1, 2]. These patterns involve three different power law regimes and a quasi-universality on the phase-shift parameter rho: 2kR(m-1), where R is the radius and m the refractive index. Similar patterns appear for non-spherical particles. These patterns give us an empirical description of scattering by particles of arbitrary shape and refractive index. In other work we have explored the consequences of symmetry or its lack on polarization and backscattering. These results can be useful for predicting the scattering of atmospheric aerosol particles. [1] C.M. Sorenson and D.F. Fischbach, Opt. Commun. 173,145 (2000). [2] M.J. Berg, C.M. Sorenson, and A. Chakrabarti, Applied Optics 44, 7487-7493 (2005). I acknowledge very useful collaborations with M. Berg and A. Chakrabarti.

4:18PM W26.00006 Understanding aerosol-cloud interactions. ATHANASIOS NENES, Schools of Earth & Atmospheric Sciences and Chemical & Biomolecular Engineering, Georgia Institute of Technology — The effects of aerosols on clouds (known as the “aerosol indirect climatic effect”) are thought to have a net climatic cooling effect which partially offsets greenhouse gas warming. Regional impacts of aerosols on precipitation and cloudiness can be even stronger. Despite its importance, the complex and multi-scale nature of aerosol-cloud interactions makes quantitative assessments of the indirect effect one of the most uncertain components of anthropogenic climate change. This talk will present the approaches used to observationally study them and represent them in models. We will provide an assessment of what has been learned and point out key research challenges for the future.
4:54PM W26.00007 Alkyl Polyoxyethylene Surfactant Residue Distribution after Sessile Droplet Evaporation. H. YUNJI MI, Albany State University, HEPING ZHU, USDA Agricultural Research Service, KWAICHOW CHAN COLLABORATION, HE Ping ZHU COLLABORATION — Post-evaporation residues of an Alkyl Polyoxyethylene surfactant on a slightly hydrophilic surface are studied. An edge-detecting contrast recognition algorithm is used to measure the areas of small (7-30µm diameter) surfactant “islands” which form during the evaporation process as a result of flows within the droplet and surface tension gathering. “Island” distributions broaden with increased concentration, accompanied by higher mean interior island size. Fitting the histogram of island sizes beginning with the principle peak reveals a general form: \( y = (6 \times 10^{-6}) C x^{-1.5} \) where \( y \) is frequency, \( C \) the concentration and \( x \) is a constant having value between 2.55 and 3.00. Log-log plots evidence a linear behaviour over two orders of magnitude. Total area covered does not increase in a linear fashion with concentration, as one may expect. Rather, a “critical” concentration is achieved at approximately 0.15%, above which area increase is less pronounced.

1 Funding was made possible (in part) by 5P20MD000108-04 from the National Ctr on Minority Health and Health Disparities. Views expressed are the presenter’s, and do not constitute endorsement by DHHS.

5:06PM W26.00008 ABSTRACT WITHDRAWN

Thursday, March 13, 2008 2:30PM - 5:18PM
Session W27 GMAG: Focus Session: Spin Glasses and SrCu\(_2\)(BO\(_3\))\(_2\)

5:20PM W27.00001 Unconstrained Chern-Simons theory for the geometrically frustrated spin compound SrCu\(_2\)(BO\(_3\))\(_2\) . CRISTIAN BATISTA, PINAKI SENGUPTA, LANL, SUCHITRA SEBASTIAN, Univ. of Cambridge, NEIL HARRISON, LANL — We show that an unconstrained Chern-Simons theory – where the local densities are determined in a self-consistent manner – correctly reproduces the sequence of magnetization plateaus recently observed in the geometrically frustrated spin compound SrCu\(_2\)(BO\(_3\))\(_2\) in an external magnetic field. The theory predicts that at the plateaus, the triplets are arranged in stripe patterns which is consistent with NMR experiments at and close to the 1/8 plateau.

5:42PM W27.00002 Fractalisation drives crystalline states in the frustrated spin system SrCu\(_2\)(BO\(_3\))\(_2\) . SUCHITRA SEBASTIAN, Cambridge University, N. HARRISON, P. SENGUPTA, C.D. BATISTA, S. FRANCOUAL, NHMFL, Los Alamos National Laboratory, E. PALM, T. MURPHY, NHMFL, Tallahassee, H.A. DABKOWSKA, B.D. GAULIN, McMaster University — Geometrical frustration in the spin dimer material SrCu\(_2\)(BO\(_3\))\(_2\) leads to a singlet Shashty-Sutherland groundstate at low magnetic fields, but complex spin superstructures at higher fields. Our magnetisation measurements reveal a fine substructure of quantum Hall-like plateaux at all 1/q ratios 2 < q < 9 and p/q = 2/9 in magnetic fields up to 85 T and temperatures down to 29 mK, within the sequence of previously identified plateaux at 1/8, 1/4, and 1/3 of the saturated magnetisation. We identify this hierarchy of plateaux as a consequence of confined bosons in SrCu\(_2\)(BO\(_3\))\(_2\) mimicking the high magnetic field fractalisation predicted by the Hofstadter butterfly for fermionic systems. Such an experimental realisation of the Hofstadter butterfly has not been previously achieved in real interacting materials, given the unachievably high magnetic fluid flux densities or large lattice periods required. By a theoretical treatment that includes short-range repulsion in the Hofstadter treatment, stripe-like spin density-modulated phases are revealed in SrCu\(_2\)(BO\(_3\))\(_2\) as emergent from a fluidic fractal spectrum.

6:00PM W27.00003 Doped Valence Bond Solid and Superconductivity on the Shastry-Sutherland Lattice . BOHM-JUNG YANG, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, YONG BAEK KIM, Department of Physics, University of Toronto, Toronto, Ontario, Canada, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, KWON PARK, School of Physics, Korea Institute for Advanced Study, Seoul, Korea — Motivated by recent experiments on SrCu\(_2\)(BO\(_3\))\(_2\), we present a theoretical framework for understanding the ground states of the doped Mott insulator on the Shastry-Sutherland lattice. To provide a unified theoretical framework for both the valence bond solid state found in undoped SrCu\(_2\)(BO\(_3\))\(_2\) and the doped counterpart in on-going experimental pursuit, we analyzed the \( t-J-V \) model via the bond operator formalism. The interplay between strong dimerization and the nearest-neighbor repulsive interaction leads to different behaviors of the doped holes determining the overall phase diagram. Specifically, if the nearest-neighbor repulsive interaction, \( V \), is smaller than a critical value, \( V_c \), the hole-pairing within dimers is preferred, resulting in the \( S \)-wave superconductivity at any non-zero \( x \). On the other hand, if \( V \) is larger than \( V_c \), the density of paired-holes within the same dimers vanishes at finite \( x \) and the plaquette \( D \)-wave superconductivity with a peculiar spatial pattern emerges. Implications to future experiments are discussed.

6:20PM W27.00004 Critical Properties of the Unconventional Spin-Peierls System TiOBr . J.P. CLANCY, B.D. GAULIN, Department of Physics and Astronomy, McMaster University, F.C. CHOU, Center for Condensed Matter Sciences, National Taiwan University — TiOBr is one of only three inorganic compounds which have been shown to undergo a spin-Peierls (SP) transition, developing a dimerized singlet sequence of magnetization plateaus recently observed in the geometrically frustrated spin compound SrCu\(_2\)(BO\(_3\))\(_2\) as emergent from a fluidic fractal spectrum.

3:18PM W27.00005 Thermal properties and Ehrenfest relation in an “ideal” spin glass. S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory/Iowa State University, G.M. SCHMIEDESHOFF, Department of Physics, Occidental College — In order to test whether the Ehrenfest relation is applicable to the spin glass “transition,” we report temperature-dependent heat capacity and thermal expansion measurements on an “ideal” spin glass material: single grain isocohedral Gd-Mg-Zn quasicrystal and its non-magnetic counterpart, Y-Mg-Zn. Spin-glass state related signatures are clearly seen in the Gd-Mg-Zn data sets. Directly measured pressure dependence of the freezing temperature in Gd-Mg-Zn is compared to its evaluation through the Ehrenfest relation.

1 Supported by US DOE BES DE-AC02-07CH11358 and NSF DMR-0704406.
3:30PM W27.00006 Anomalous field-sweep rate dependence of magnetization process of a spin-glass system Fe$_{1-x}$Mn$_x$TiO$_3$. N. MIURA, H. ARUGA KATORI, A. ITO, RIKEN, M. SCHOENHART, R. GROESSINGER, Tech. Univ. Vienna, N. V. KOZLOVA, K. DOERR, IFW, Dresden, RIKEN TEAM, VIENNA TEAM, IFW TEAM — A mixed compound Fe$_{60-x}$Mn$_x$TiO$_3$ is a typical ising spin-glass. When a magnetic field is applied to the spin-glass state with a rather fast sweep rate 0.2 < dB/dt < 1 T/s by a steady field magnet, the sample shows step-like jumps in the magnetization, whereas in a pulse magnet with an even faster sweep rate above 700 T/s, it shows a smooth metamagnetic transition. The field of the step-like jump is decreased as the sweep rate is increased, which is contrary to any relaxation phenomena with a slow response time. In the case of smooth metamagnetic transition at faster sweep rates, the transition field is increased as the sweep rate is increased. In this study, we investigated the magnetization process in the intermediate range of field sweep rate between 1.0 and 124 T/s using an ultra-long-pulse magnet. It was found that as the sweep rate is increased, the jump behavior changes over to the metamagnetic behavior at around 2.5 T/s, where the transition field takes the minimum. The observed results are suggestive of some locally grown non-equilibrium spin alignment. The jump behavior is discussed in connection with similar phenomena in perovskite manganites.

3:42PM W27.00007 The Free Energy Landscape of a Two-Dimensional Spin Glass from a Hard- Spin Mean-Field Treatment, MICHAEL MIHALCO, SUSAN MCKAY, University of Maine — The two-dimensional Ising antiferromagnet on a triangular lattice shows no ordered phase at finite temperatures until frustration is relieved, often accomplished through dilution (Grest and Gabl PRL 43, Netz and Berker PRL 66) or by the addition of randomly placed ferromagnetic bonds. Using the second approach, we have created a two-dimensional spin-glass phase with tunable frustration and explored its free energy landscape using a hard-spin mean-field approach (Netz and Berker PRL 66). The Monte Carlo implementation of this method quickly provides a self-consistent solution of site magnetizations, and we have used the overlaps and internal energies of various solutions to explore the energy landscape as a function of temperature and the number of frustrated plaquettes. Results indicate a multiplicity of solutions and a rich structure of overlaps, which are sensitive to the temperature and level of frustration. This method shows clearly the distinctions between the spin-glass phase and the bordering ferromagnetic ordering that occurs once the ferromagnetic interactions dominate.

3:54PM W27.00008 Field-Driven Hysteresis of the d=3 Ising Spin Glass: Hard-Spin Mean-Field Theory, BURCU YÜCESOY, Istanbul Technical University and University of Massachusetts, Amherst, A. NIHAT BERKER, Koç University — Hysteresis loops are obtained in the Ising spin-glass phase in d = 3, using frustration-conserving hard-spin mean-field theory.[1] The system is driven by a time-dependent random magnetic field $H(t)$ that is conjugate to the spin-glass order $Q$, yielding a field-driven first-order phase transition through the spin-glass phase. The hysteresis loop area $A - A_0$ scales with respect to the sweep rate $h$ of magnetic field as $A - A_0 \sim h^\beta$. In the spin-glass and random-bond ferromagnetic phases, the sweep-rate scaling exponent $\beta$ changes with temperature $T$, but appears not to change with antiferromagnetic bond concentration $\rho$. By contrast, in the pure ferromagnetic phase, $\beta$ does not depend on $T$ and has a sharply different value than in the two other phases.

4:06PM W27.00009 Quantum Induced Asymmetric Phase Diagrams of Spin-Glass Systems, C. NADIR KAPLAN, A. NIHAT BERKER, Koç University — The spin-1/2 quantum Heisenberg spin-glass system is studied in all spatial dimensions $d$ by renormalization-group theory.[1] Strongly asymmetric phase diagrams in temperature and antiferromagnetic bond probability $p$ are obtained in dimensions $d \geq 3$. The asymmetry at high temperatures approaching the pure ferromagnetic and antiferromagnetic systems disappears as $d$ is increased. However, the asymmetry at low but finite temperatures remains in all dimensions, with the antiferromagnetic phase receding to the ferromagnetic phase. A finite-temperature second-order phase transition is obtained in the antiferromagnetic and spin-glass phases occur in $d \geq 6$, resulting in a new multicritical point at its meeting with the boundaries to the paramagnetic phase. In $d = 3, 4, 5$, a paramagnetic phase reaching zero temperature intervenes asymmetrically between the ferromagnetic and antiferromagnetic phases. There is no spin-glass phase in any dimension.

4:18PM W27.00010 Spin phonon induced colinear order and magnetization plateaus in triangular and kagome antiferromagnets. Applications to CuFeO$_2$, FA WANG, ASHVIN VISHWANATH, Department of Physics, University of California at Berkeley; Material Sciences Division, Lawrence Berkeley National Laboratory — Coupling between spin and lattice degrees of freedom is important in geometrically frustrated magnets where they can lead to degeneracy lifting and novel orders. We show that moderate spin-lattice couplings in triangular and Kagome antiferromagnets can induce complex colinear magnetic orders. When classical Heisenberg spins on the triangular lattice are coupled to Einstein phonons, a rich variety of phases emerge, including the experimentally observed four sublattice state and the five sublattice 1/5th magnetization plateau state seen in the magneto-electric material CuFeO$_2$. In addition we predict magnetization plateaus at 1/3, 3/7, 1/2, 3/5 and 5/7 at these couplings. Strong spin-lattice couplings induce a striped colinear state, seen in α-NaFeO$_2$ and MnBr$_2$. On the Kagome lattice, moderate spin-lattice couplings induce colinear order, but an extensive degeneracy remains.

4:30PM W27.00011 Jahn-Teller coupling and magnetic ground state in vanadium spinels, GIA-WEI CHERN, OLEG TCHERNYSHYOV, Johns Hopkins University — The interplay of orbital, lattice, and spin degrees of freedom in vanadium spinels has attracted much interest among researchers. The V$^{4+}$ ion has two electrons occupying three degenerate $t_{2g}$ orbitals and is thus Jahn-Teller active. It also has a total spin $S = 1$ in accordance with Hund’s rules. Moreover, the V$^{4+}$ ions sitting on the B-site of spinel form a pyrochlore lattice, the interactions between these localized spin and orbital degrees of freedom are thus geometrically frustrated.[1] Here we present a theoretical model for the ground states of vanadium spinels. We view all of the vanadates (Cd, Zn, Mg on the one hand and Mn on the other) within the same model in which the influence of Mn is simulated by magnetic field as $A - A_0 \sim h^\beta$. In the spin-glass and antiferromagnetic phases occur in $d \geq 6$, resulting in a new multicritical point at its meeting with the boundaries to the paramagnetic phase. In $d = 3, 4, 5$, a paramagnetic phase reaching zero temperature intervenes asymmetrically between the ferromagnetic and antiferromagnetic phases. There is no spin-glass phase in any dimension.

4:42PM W27.00012 AC Susceptibility and Heat Capacity Studies of Geometrically Frustrated Pyrochlores, DANIEL ANTONIO, ANDREW CORNELIUS, UNLV, JASON GARDNER, Brookhaven National Lab, NIST — Materials with a geometrically frustrated pyrochlore lattice have been of interest due to their unusual ground states. Tb$_2$Ti$_2$O$_7$ is known for going to a spin liquid ground state and does not transition to a long-range ordered state down to at least 50 mK [1]. Ho$_2$Ti$_2$O$_7$ has a macroscopically degenerate spin ice ground state which resembles that of the proton ordering in water ice [2]. Heat Capacity measurements of Tb$_2$Ti$_2$O$_7$ were done from 300 K to 0.36 K and AC magnetic susceptibility measurements of Ho$_2$Y$_2$Ti$_2$O$_7$ and Zr$_2$La$_2$Ti$_2$O$_7$ were done for frequencies from 10 Hz to 10 kHz down to 1.8 K, both in magnetic fields up to 9 T. These experiments were performed to further understand the factors leading to their unusual behavior and the effects of introducing disorder through doping with nonmagnetic elements. Determination of the effect of an external field on the hyperfine crystal field at the Tb sites was done. In addition, unusual behavior in the ac susceptibility of the Ho samples at lower temperatures was observed.[1] J.S. Gardner et al., Phys. Rev. Lett. 82, 1012 (1999)[2] S.T. Bramwell and M.J.P. Gingras, Science 294, 1495 (2001)
4:54PM W27.00013 Local studies of AC demagnetization in a model frustrated magnet. JIE LI, XIAOLIN KE, CRISTIANO NISOLI, PAUL LAMMERT, VINCENT CRESPI, PETER SCHIFFER, The Penn State Univ. — We have studied the process of ac demagnetization using a model system consisting of single-domain ferromagnetic islands arranged on perpendicular square lattices such that the interaction between the islands is frustrated by the geometry of the arrays. The sample is first subjected to an oscillating magnetic field whose magnitude is stepped down by different step sizes and the sample is rotating at the same time. We find that the net moment of the arrays can be readily brought to near zero with the magnetic field step size below a certain threshold value. However the interaction energy of the demagnetized array state continues to decrease linearly with decreasing step size even as the step size approaches zero. We characterize the result in terms of developing local correlations between the island moments, with strong analogies to other athermal magnetic systems. This research has been supported by the Army Research Office.

3This research has been supported by the Army Research Office.

5:06PM W27.00014 Dimensional Crossover in ZnMn$_2$O$_4$. WILLIAM RATCLIFF, National Institute of Standards and Technology (NCNR), YING CHEN, GORAN GARASPOVIC, YIMING QIU, National Institute of Standards and Technology (NCNR), U. Maryland (Materials Science and Engineering), QING HUANG, JEFFREY LYNN, National Institute of Standards and Technology (NCNR), SUNMOG YEO, Rutgers University (Department of Physics), SANG CHEONG, Rutgers University (Department of Physics), PAULA PICCOLI, ARTHUR SCHULTZ, Argonne National Lab (IPNS) — ZnMn$_2$O$_4$ crystallizes at high temperatures as a cubic spinel. At lower temperatures, it undergoes a Jahn Teller distortion which lowers its symmetry to tetragonal. At lower temperatures (TN~60 K), the system orders magnetically. Fits to the order parameter, line shape of powder diffraction peaks, and the direct observation of rods of scattering in single crystal diffraction experiments show the system to be two dimensional. This is likely due to the interplay between orbital ordering and frustration. In this talk I discuss the magnetic structure and spin waves of this system. I will also discuss an interesting crossover in the dimensionality of the magnetism in this compound.

Thursday, March 13, 2008 2:30PM - 5:18PM —
Session W28 DCMP: Superlattices and Nanostructures: Electronic Properties II Morial Convention Center 220

2:30PM W28.00001 Tunnel spectroscopy in an ac-driven triple dot quantum shuttle. J. VILLAVICENCIO, Universidad Autónoma de Baja California, México, I. MALDONADO, Centro de Investigación Científica y de Educación Superior de Ensenada, México, R. SÁNCHEZ, Instituto de Ciencia de Materiales de Madrid-CSIC, Spain, E. COTA, Universidad Nacional Autónoma de México, México, G. PLATERO, Instituto de Ciencia de Materiales de Madrid-CSIC, Spain — Within the framework of a fully quantum mechanical approach we use the density matrix master equation formalism to study the electronic transport in a triple dot quantum shuttle in the presence of an ac-field. We show that the ac-field induces photos-assisted tunneling which manifests itself as sidebands in the electronic current. We also show that these new tunneling sidebands can be explained in terms of simple sum rules involving the number of absorbed and emitted photons and the oscillator states participating in the process. Finally, we demonstrate that the tunneling channels can be controlled by manipulating the frequency and intensity of the ac-field, giving rise in particular to coherent destruction of tunneling (CDT).

3Work supported by: MCYT, Spain (MAT2005-06444), EU Programme (HPRN-CT-2000-00144), MEYC, Spain (SB2005-0047), and CONACYT, México (43673-F).

2:42PM W28.00002 Fabrication and Characterization of a CMOS-Based Quantum Dot Device. MING XIAO, E. YABLONOVITCH, H.W. JIANG, UCLA — Silicon-based single electron devices are particularly attractive for implementing quantum information processing due to the extremely long electron spin lifetimes. We report here the demonstration of a stack-gated CMOS structure that can define a quantum dot in the few-electron regime with a sensitive, high bandwidth field effect transistor. Multiple lower layer side gates, as small as 50nm, on an ion-implanted Si/SiO2 wafer electrostatically define the quantum dot. A top gate that controls the electron population in the quantum dot is then fabricated on top of an isolating AlO3 layer made by atomic layer deposition (ALD). The low-temperature ALD process provides excellent device stability and preserving the integrity of the side gates. We found that the devices can be operated effectively both in the accumulation mode and in the depletion mode. Transport through the quantum dots in the few-electron regime for currents less than 100fA can be reliably studied with a good reproducibility. We will detail our fabrication and characterization processes in this presentation.

2:54PM W28.00003 Transport through a triple quantum-dot ring in high-spin state. YUNORI NISIKAWA, Osaka City University, TAKAHIDE NUMATA, AKIRA OGURI, Osaka City University — Using the numerical renormalization group (NRG), we study transport through a triple quantum-dot ring in high-spin state, connected to two noninteracting leads symmetrically. The transport is determined by two phase shifts for quasi-particles with even and odd parities. An isolated triple quantum-dot ring has a high spin ground state of S = 1 caused by a Nagaoka ferromagnetism, when it has one extra electron introduced into a half-filling. The results show that the conduction electrons screen the local moment within two separate stages with different energy scales. The half of the S = 1 is screened first by one of the channel degrees, and then at very low temperature the remaining half is fully screened to form a Kondo singlet. A two-terminal conductance in the series configuration is suppressed similar or equal to 0, while plateau of a four-terminal parallel conductance reaches a unitary limit value similar or equal to 4e^2/h of two conducting modes. We also present the relation between electronic states and thermodynamic quantities calculated using NRG eigen energies.

3:06PM W28.00004 Valley Splitting in Different Landau Levels of a Si/SiGe Quantum Point Contact. LISA McGUIRE, University of Wisconsin-Madison, K.A. SLINKER, MARK FRIESEN, University of Wisconsin-Madison, SRIJIT GOSWAMI, J.O. CHU, IBM Research Division-T.J. Watson Research Center, ROBERT JOYNT, S.N. COPPERSMITH, MARK A. ERIKSSON, University of Wisconsin-Madison — Si/SiGe is an interesting platform for spin physics and quantum information due to the weak spin-orbit coupling in Si and the presence of nuclear spin zero isotopes. However, silicon has a near degeneracy of orbital states in the conduction band arising from multiple valley minima, which could enhance decoherence rates and complicate qubit operation. Recent measurements in a quantum point contact have shown that the valley splitting is large, of order 0.5 ~ 2 meV. Here, we investigate fundamental mechanisms of valley splitting by taking into account the valley couplings between Landau levels. We also account for the dependence of valley splitting on materials parameters such as miscut angle and device orientation. From our data, we are able to extract distinct valley splittings from the lowest two Landau levels, which vary similarly as a function of gate voltage (i.e., channel width). We are further able to place bounds on local variations of the tilt angle of the quantum well interface. Work supported by ARQ, NSA, and NSF. 1 S. Goswami et al., Nature Physics 3 (1): 41-45 JAN 2007.
3:18PM W28.00005 Counting statistics and conditional evolution in a quantum electromechanical system, STEVEN BENNETT, AASHISH CLERK, McGill University — We present a theoretical study of full counting statistics (FCS) and conditional evolution of a quantum point contact (QPC) coupled to a mechanical oscillator. Such a system has recently been studied in several experiments. Starting from a microscopic model, we derive a master equation for the reduced density matrix that contains several important differences from the usual equation used to describe conditional position evolution (i.e., the dynamics of the oscillator inferred from a particular measurement outcome of current through the QPC). The master equation may then be solved analytically to obtain the FCS and conditional evolution. We find that the oscillator can significantly affect the FCS, leading to a highly non-Gaussian distribution characterized by an enhanced third moment even for very weak coupling. In the conditional evolution we find clear evidence that the back-action of the QPC on the oscillator cannot simply be described as coupling to an effective thermal bath.

3:30PM W28.00006 Thermo-electric effects in nanostructures out of equilibrium, YONATAN DUBI, ROBERTO D’AGOSTA, MASSIMILIANO DI VENTRA, University of California-San Diego — As technology advances into the nanoscale regime, probing the electronic properties of nanoscale circuits has become a major challenge. Specifically, it has been suggested that thermo-electric effects may serve as a tool to study electronic properties of nanoscale systems, and experiments on thermo-power in quantum point contacts (QPCs) and molecular circuits have been performed. On the theoretical side, however, linear-response theory is inadequate to determine the dynamical formation of the thermo-electric effect. Here, we propose a novel scheme to calculate dynamical thermo-electric effects in nanostructures arbitrarily far from equilibrium using a local generalization of the Lindblad master equation. We demonstrate the method by calculating the charge imbalance of a QPC in the presence of Coulomb interactions and a temperature gradient, and obtain the long-time energy distribution in the QPC out of equilibrium. Our suggested scheme can be implemented into stochastic time-dependent current-density functional theory [PRL, 98, 226403 (2007)], thus providing a valuable tool in studying the interplay of charge and energy currents for arbitrary many-body systems.

3:42PM W28.00007 Universality and the thermal dependence of the conductance of nanodevices, LUIZ N. OLIVEIRA, Univ. Sao Paulo, ANTONIO C. SERIDONIO, Univ. Brasilia, MAKOTO YOSHIDA, Univ. Estadual Paulista — The conductance of a quantum wire side-coupled to a quantum dot will be discussed. In this device, plots of the conductance $G$ vs. the gate voltage $V_g$ applied to the dot display Fano antiresonances due to the interference between the current traversing the wire and the flux of electrons that hop to the dot to bypass the adjacent section of the wire; at fixed $V_g$'s, the interference accounts for a variety of thermal dependences $G(T)$. Analytical renormalization-group arguments will be presented that map $G(T)$ to the universal curve $g(T/T_K)$ for the conductance of the spin-degenerate Anderson impurity Hamiltonian, with temperatures normalized by the Kondo temperature $T_K$. This linear, universal mapping will be shown to (i) generate curves in excellent agreement with the measurements of Sato et al. [Phys. Rev. Lett. 95, 066801 (2005)] and justify those authors' phenomenological description of their data; (ii) fit novel numerical renormalization-group data for the conductance of the side-coupled device; and (iii) link $G(T)$ to the conductance of the single-electron transistor.

1Work supported by DOE.

3:54PM W28.00008 Electronic Properties of Quantum Point Contacts in a Quantum Ring, A. DEVRIM GUCLU, Duke University, CYRUS J. UMIRGAR, Cornell University, HAROLD U. BARANGER, Duke University — We investigate the electronic properties of a narrow constriction (quantum point contact) in a quantum ring using variational and diffusion Monte Carlo methods. Quantum point contacts are basic building blocks of nanoscale devices. The experimental control over their width allowed the observation of conductance quantization in integer steps of $G_0 = 2e^2/h$. However, a puzzling additional structure is also observed around $0.7G_0$ in some devices. One possible explanation is the formation of a local quasi-bound state. Here, we present a first quantum Monte Carlo calculation showing that electrons can be strongly localized in the constriction, with a well quantized electron number $N$ that varies abruptly as the width of the point contact decreases. We also study the low-lying excited states and investigate the possibility of a spin texture as a function of applied gate voltage.

4:06PM W28.00009 Piezoelectric models for semiconductor quantum dots, MORTEN WILLATZEN, BENNY LASSEN, DANIELLE BARETTIN, University of Southern Denmark, LOK LEW YAN VOON, Wright State University, UNIVERSITY OF SOUTHERN DENMARK COLLABORATION, WRIGHT STATE UNIVERSITY COLLABORATION — The importance of fully-coupled and semi-coupled piezoelectric models for quantum dots will be presented and compared to corresponding results for one-dimensional heterostructures. Electron energies differences of up to around 30 meV were found possible for GaN/AlN quantum dots.

1Acknowledgment support from Research and Sponsored Office, Wright State University and Banff International Research Station.

4:18PM W28.00010 High sensitivity cantilevers for measuring persistent currents in normal metal rings, ANIA BLESZYNJSKI JAYICH, WILL SHANKS, Yale University, ROB ILIC, Cornell University, JACK HARRIS, Yale University — We propose a new approach to measuring persistent currents in normal metal rings. By integrating micron-scale metal rings into sensitive micromechanical cantilevers and using the cantilevers as torque magnetometers, it should be possible to measure the rings' persistent currents with greater sensitivity than the SQUID-based and microwave resonator-based detectors used in the past. In addition, cantilever-based detectors may allow for measurements in a cleaner electromagnetic environment. We have fabricated ultra sensitive cantilevers with integrated rings and measured their mechanical properties. We present an estimate of the persistent current sensitivity of these cantilever-based detectors, focusing on the limits set by the cantilever's Brownian motion and the shot noise in the laser interferometer that monitors the cantilever.

4:30PM W28.00011 Electron Pair Resonance in the Coulomb Blockade, MIKHAIL RAIKH, University of Utah, ERAN SELA, University of British Columbia, HEUNG-SUN SIM, Korea Advanced Institute of Science and Technology, YUVAL OREG, Weizmann Institute of Science, FELIX VON OPPEN, Free University of Berlin — Transport through a nanostructure in the regime of Coulomb blockade is dominated by elastic single-electron cotunneling. We study many-body corrections to the cotunneling current via a localized state with energy $e_0$ at large bias voltages $V$. We show that the transfer of electron pairs, enabled by the Coulomb repulsion in the localized level, results in ionization resonance peaks in the third derivative of the current with respect to $V$, centered at $eV = \pm 2e_0/3$. Our results predict the existence of previously unnoticed structure within Coulomb-blockade diamonds. Remarkably, this new structure emerges within the standard Anderson Hamiltonian conventionally used for description of transport through nanostructures.
4:42PM W28.00012 Quantum Dot Array for Simulating the Hubbard Model, CHING-TZU CHEN, DENNIS M. NEWNS, CHANG C. TSUET, IBM Thomas J Watson Research Center, JEFFREY J. URBAN, The Molecular Foundry, Lawrence Berkeley National Lab — As the simplest theory that incorporates strong onsite Coulomb repulsion, the Hubbard model is fundamental to the understanding of phenomena in strongly correlated systems, e.g. the metal-insulator transition in transition-metal oxides. It is widely believed that the 2D square-lattice Hubbard model captures the puzzling physics of high-temperature superconductivity. Since an analytical solution of the model is not viable, we propose to study its properties through a “quantum simulator” made from quantum dot arrays (QDAs). In this talk, we first demonstrate the correspondence between the Hubbard Hamiltonian and the simplified model for the QDA. We then address the scaling of the crucial parameters for designing a practical simulator. Two systems for implementing the QDA are proposed — the self-assembled nanocrystal arrays, and the lithographically defined 2D-electron-gas QDA. Preliminary experimental results derived from these systems will be presented.

4:54PM W28.00013 Correlation effects with low electron density along a potential barrier in quantum point contacts. KARAN ARYANPOUR, JONG HAN, Department of Physics, SUNY at Buffalo — We study correlated electrons effect in the conductance through Quantum Point Contacts (QPC). Conductance of a QPC is quantized in steps of $G_0 = \frac{2e^2}{h}$ (e the charge of an electron and h Planck's constant). Experiments also reveal an additional neutral shoulder near $0.7G_0$ referred to as the 0.7 anomaly. Evidence supporting spin 1/2 magnetic moment formation in the conductance channel has motivated scenarios such as the Kondo effect. We intend to address whether or not the 0.7 anomaly is a many-body effect associated with the formation of a spin 1/2 magnetic moment in the conductance channel. We employ the Quantum Monte Carlo (QMC) technique for electrons on a 1-D QPC lattice with an adiabatic potential barrier. The QPC lattice includes the Hubbard lattice in the QPC region and two leads modeled by semi-infinite chains and we calculate the conductance along the chain using the Kubo formula. The physics is determined by the competition between the many-body interaction and the small kinetic energy at the top of the potential barrier. Due to the singular nature of the density of states at low electron density along with the spatial inhomogeneity, the many-body effects are expected to differ from conventional wide-band limit physics.

Thursday, March 13, 2008 2:30PM - 5:30PM — Session W29 DMP: Focus Session: Carbon Nanotubes and Related Materials XIV: Theory and Sensing Morial Convention Center 221

2:30PM W29.00001 Electron-phonon interaction and excited states relaxation in carbon nanotubes. VASILI PEREBEINOS, IBM - Watson — We will discuss the role of electron-phonon interaction on excited states relaxation and phonon spectra in carbon nanotubes (CNTs). The electron-phonon interaction leads to the polaronic effects of the charge carriers, but it also renormalizes the energy and the lifetime of phonons. We present a theoretical model that predicts the changes induced in the phonon modes of CNTs as a function of the charge carrier doping, i.e. position of the Fermi level. In agreement with the predictions, our experiments show sharpening and blue shifts of the G-phonons of metallic CNTs, but only blue shifts for semiconducting CNTs, making the Raman scattering a useful probe of local doping of CNTs. In the reverse process of photoconductivity, light is absorbed creating excited states. We will discuss electronic relaxation of high energy excited states leading to the strong impact excitation and light emission, which intensity is determined by electric field, phonon scattering, and impact excitation cross section.

3:06PM W29.00012 Study of Butane adsorption on Purified HiPco Carbon Nanotubes. TOYO FURUHASHI, DINESH RAWAT, ALDO MIGONE, Southern Illinois University, Carbondale, IL-62901 — We investigated the adsorption characteristics of butane on purified HiPco single-walled carbon nanotubes for coverages in the first layer. We measured 9 full isotherms between 180 and 260K. The results for butane are compared with those obtained in a previous study of ethane adsorption on the same substrate. Comparable values for the specific surface area of the substrate were found when this quantity was measured using either ethane or butane. This strongly suggests that both of these species have access to essentially the same adsorption sites. We also determined that the strength of binding of the hydrocarbon chains to the SWNT bundles correlates, roughly linearly, with molecular length. An increase in chain length provides a greater number of contacts between sites on the substrate and the adsorbate species, thus, resulting in an increase in the values of the binding energies.

3:06PM W29.00002 Study of Butane adsorption on Purified HiPco Carbon Nanotubes. TOYO FURUHASHI, DINESH RAWAT, ALDO MIGONE, Southern Illinois University, Carbondale, IL-62901 — We investigated the adsorption characteristics of butane on purified HiPco single-walled carbon nanotubes for coverages in the first layer. We measured 9 full isotherms between 180 and 260K. The results for butane are compared with those obtained in a previous study of ethane adsorption on the same substrate. Comparable values for the specific surface area of the substrate were found when this quantity was measured using either ethane or butane. This strongly suggests that both of these species have access to essentially the same adsorption sites. We also determined that the strength of binding of the hydrocarbon chains to the SWNT bundles correlates, roughly linearly, with molecular length. An increase in chain length provides a greater number of contacts between sites on the substrate and the adsorbate species, thus, resulting in an increase in the values of the binding energies.

3:18PM W29.00003 Adsorption Kinetics of CH4 on Purified HiPco Single-Walled Carbon Nanotubes. MURAT BULUT, DINESH S. RAWAT, ALDO D. MIGONE, Southern Illinois University Carbondale — We present the results of an adsorption kinetics study of CH4 on two sets of purified HiPco SWNTs. We monitor the time evolution of the pressure from the instant at which gas is added to the cell containing the nanotubes to the moment at which equilibrium is reached. The two sets of samples were baked, under vacuum, at different temperatures (300 and 400°C). The difference in baking temperatures resulted in a difference in the specific surface areas; the sample treated at 400°C has a 15% larger surface area than the sample treated at 300°C. It also caused a difference in the kinetic behavior of the samples; the equilibration times for the two samples differ by a factor of 3. Moreover, the sample heated at 400°C exhibits two distinct equilibration times, while the one heated at 300°C exhibits only one. These changes are probably the result of partially opening the purified SWNTs by baking them at 400°C, which does not occur when we heat them only to 300°C.

This work was supported by NSF through grant # DMR-0705077.
3:30PM W29.00004 Adsorption kinetics of diatomic molecules on carbon nanotube bundles. JARED BURDE, MERCEDES CALIBI, Dep. of Physics, Southern Illinois Univ. Carbondale — A Kinetic Monte Carlo algorithm is used to explore the kinetics of adsorption of diatomic adsorbates on one-dimensional chains of sites. In particular, we monitor the evolution of the orientational configuration of the adsorbate as equilibrium is being reached at different values of temperature and chemical potential. We also analyze the dependence of the orientational evolution of the phases on the interactions between the molecules and on the presence of adsorption sites with different energies.

3:42PM W29.00005 Equilibration times of adsorption on external surfaces of carbon nanotube bundles. NAYELI ZUNIGA, Dep. of Physics, Southern Illinois Univ. Carbondale, JARED BURDE, MERCEDES CALIBI, ep. of Physics, Southern Illinois Univ. Carbondale — We investigate the adsorption kinetics of gases on the exterior of a carbon nanotube bundle by monitoring the uptake and exchange of particles in regions of the surface characterized by different binding energies. By using a Kinetic Monte Carlo scheme, we follow the time evolution of the gas uptake for different values of external pressure and temperature. The presence of adsorption sites with different energies gives rise to distinctive features on the equilibration time as function of the coverage. We show that preliminary experimental results for CF4, Ar, and CH4 on nanotube bundles with closed ends are consistent with our results.

3:54PM W29.00006 Adsorption kinetics of binary mixtures on carbon nanotube bundles. SEYOUNG TSIGE, JARED BURDE, MERCEDES CALIBI, Dep. of Physics, Southern Illinois Univ. Carbondale — We examine kinetic selectivity effects that take place during the adsorption of a binary mixture on one-dimensional chains. After reaching equilibrium at the same chemical potential, the species with the higher binding energy will enjoy the greatest coverage. However, the weaker-binding species has faster adsorption kinetics and is able to reach a coverage higher than its equilibrium value before the stronger species can adsorb significantly. The result of this process is an ‘overshoot’ in the fractional coverage of the weaker species that is reached at a time long before the system equilibrates. We analyze the appearance of this overshoot as a function of the temperature, chemical potentials, and energy parameters of the system.

4:06PM W29.00007 Hydrogen sensing properties of palladium-decorated carbon nanotube circuits. VAIKUNTH KHALAP, TATYANA SHEPS, ALEXANDER KANE, PHILIP COLLINS — Sensitive hydrogen gas sensors can be fabricated from carbon nanotube circuits decorated with palladium metal, and we have investigated the responsible physical mechanisms using isolated, single-walled carbon nanotubes (SWCNTs). Hydrogen sensitivity arises from two active mechanisms, neither of which is the mere adsorption of Pd onto pristine SWCNTs. The first mechanism relies on the chemical sensitivity of Schottky barriers present when semiconducting SWCNTs are contacted by metals. Pd decoration of the barrier region, or the use of pure Pd as the contact metal, produces a modest H2 sensitivity, if any. A more sensitive mechanism involves Pd-decorated defect sites, which in both metallic and semiconducting SWNTs results in reversible conductance swings of 100%. This presentation will review the temporal dynamics and pressure dependence of both mechanisms.

4:18PM W29.00008 Electrical Measurement of Single Molecule Catalysis using Carbon Nanotubes. BRETT R. GOLDSMITH, ALEXANDER A. KANE, VAIKUNTH KHALAP, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697, JOHN CORONEUS, Department of Molecular Biology and Biochemistry, University of California Irvine, Irvine, CA 92697, GREGORY A. WEISS, Departments of Chemistry, Molecular Biology and Biochemistry, University of California Irvine, Irvine, CA 92697, PHILIP G. COLLINS, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697 — We demonstrate single molecule chemical sensors based on single-walled carbon nanotubes (SWNT). The architecture uses a SWNT conductor having a single, reactive species covalently bonded to the sidewall [1]. Dynamics of the molecule are electrically transduced as it interacts with its surrounding environment. As a test case, we investigate the catalytic modification of EDC by a carboxylate. After creating a carboxylic terminus on the SWNT, the circuit is monitored for several hours and through hundreds of individual EDC reactions. Statistical analysis determines the lifetime of the carbonyl-EDC complex, as well as the catalytic turnover rate, from discrete events. Because the carboxylate site can be readily derivatized with proteins, peptides, or other functional molecules, the technique shows promise as a tool for single molecule research independent of optics and scanning probe microscopy. 1. B. R. Goldsmith, et al. Science 315, 77 (2007).

4:30PM W29.00009 Artificial introduction of defects in carbon nanotubes through Argon and Hydrogen ion irradiation, and application to chemical sensors. PRABHAKAR BANDARU, JEFFREY NICHOLS, MARK HOFER, Materials Science, UC, San Diego — The goal of this study is to quantify the effect of defect density on the electrochemical properties of multi-walled CNTs. Consequently, ion irradiation, with argon (Ar) and hydrogen (H), individually, has been performed to systematically incorporate defects into vertically aligned MWCNTs. Raman spectroscopy was used to characterize the amount of disorder within the nanotube samples. The electrochemical behavior of the irradiated MWCNT samples was then characterized through cyclic voltammetry (CV) measurements. Raman spectroscopy revealed an increase in the disorder in MWCNTs with the argon and hydrogen irradiation, as evidenced by an increase in the ID/IG peak intensity ratio. However, Ar is intercalated into the CNTs, and charges the nanotubes (forming dangling bonds), while H treatment terminates residual CNT dangling bonds. In CV, we have seen that only the Ar treated samples exhibit perfect reversible Nernstian behavior characteristic of ideal electrodes. Hydrogen treated CNT electrode ensembles seem to exhibit quicker response, as glucose sensors, with exquisite (~ 1 µM) sensitivity.

4:42PM W29.00010 Structure and thermodynamics of a Neon monolayer adsorbed on carbon nanotube bundles. OSCAR VILCHES, MICHEL BIENFAIT, Universite de la Mediterranee. MARK JOHNSTON, STEPHANE ROLS, ILI, Grenoble, SUBRAMANIAN RAMACHANDRAN, University of Washington — We report results from neutron diffraction measurements of five monolayer coverages of Ne adsorbed on single-wall, closed-end carbon nanotube bundles (SWCNB). Our recent thermodynamic study of Ne adsorbed on SWCNB, Phys. Rev. B, 76, 075404 (2007), showed one-dimensional (1d) solid behavior below 4K at doses less than 0.08 monolayer, which crossed over to 3d-like behavior above 16K without signature of a phase transition. Above 0.18 monolayer there is a 2d-like solid behavior below 8K, with Debye temperatures in the 45 to 53K range, consistent with our results. We also analyze the adsorption of a binary mixture on one-dimensional chains. After reaching equilibrium at the same chemical potential, the species with the higher binding energy will enjoy the greatest coverage. However, the weaker-binding species has faster adsorption kinetics and is able to reach a coverage higher than its equilibrium value before the stronger species can adsorb significantly. The result of this process is an ‘overshoot’ in the fractional coverage of the weaker species that is reached at a time long before the system equilibrates. We analyze the appearance of this overshoot as a function of the temperature, chemical potentials, and energy parameters of the system.

4:54PM W29.00011 Structure of a DNA-carbon nanotube hybrid using replica exchange molecular dynamics. ROBERT JOHNSON, A.T. CHARLIE JOHNSON, MICHAEL KLEIN, University of Pennsylvania — DNA-carbon nanotube hybrids (DNA-CN) are novel nanoscale materials that consist of single-wall carbon nanotubes coated with a self-assembled monolayer of single stranded DNA (ssDNA). Many recent experiments have demonstrated that this nanomaterial is an ideal candidate for a variety of nanotechnological applications. Despite the importance of this material, a complete understanding of its structural and physical properties is lacking. Recent molecular dynamics (MD) simulations of this nanomaterial have provided information about the self-assembly mechanisms and possible ssDNA conformations that characterize DNA-CN. However, MD simulations of biopolymers at low temperatures (T ~ 300 K) result in kinetic trapping and limits sampling of ssDNA configurational space. Here, we present the results of large scale replica exchange molecular dynamics simulations that provide robust sampling of the multitude of ssDNA conformations about SWCN.

3This research was supported by the JSTO, DTRA and the Army Research Office Grant # 911NF-06-1-0462. We thank the San Diego Supercomputer Center for provided generous computing time.
5:06PM W29.00012 Photon sensing with carbon nanotubes: low-temperature photothermal effect on carbon nanotube transistors, LIHONG HERMAN, ADAM TSEEN, JIWOONG PARK, Cornell University — While thermal effects on the electrical properties of carbon nanotubes (CNTs) are an area of great interest, the effect of single photons on the low temperature conductance of CNTs has not been carefully studied. We recently developed a low-temperature fiber-based laser confocal microscope with simultaneous electrical measurement capability and diffraction-limited laser illumination and detection. In our experiment, CNT devices functionalized with gold nanoparticles were illuminated with a focused laser beam while their conductance was measured at temperatures as low as 300 mK. Photon absorption by either CNTs or gold nanoparticles results in local heating and provides spatially-resolved information about the thermal effects on transport in the CNT as the laser is scanned across the device. Our technique can be easily extended to the study of single-photon effects in other nanostructures including nanowires and graphene in the near future.

5:18PM W29.00013 Transport and Charge Sensing in $^{12}$C and $^{13}$C Carbon Nanotube Double Quantum Dots¹, HUGH CHURCHILL, Harvard University, DAVID MARCOS, Harvard University/Consejo Superior de Investigaciones Cientificas, ANDREW BESTWICK, JENNIFER HARLOW, Harvard University, CAROLYN SWERTZCHA, SUSAN WATSON, Harvard University/Middlebury College, CHARLES MARCUS, Harvard University — We report measurements of gate-defined carbon nanotube double quantum dot devices with a charge sensor fabricated on the same nanotube. The methane used during growth controls the $^{13}$C content of the nanotubes. $^{12}$C nuclei have zero nuclear spin, and $^{13}$C nuclei have spin 1/2. We compare samples with natural abundance (1%) and enriched (99%) $^{13}$C content. A strong isotope effect is observed in the magnetic field dependence of transport at finite bias. Fast control of these devices is demonstrated using a pulsed-gate technique.

¹We acknowledge support from the NSF (EIA-0210736). HC acknowledges the NSF GRFP, and DM acknowledges MEC-Spain (FP/2005-0720).

Thursday, March 13, 2008 2:30PM - 5:30PM — Session W30 DMP: Nanotubes and Nanowires III: Other Properties II Morial Convention Center 222

2:30PM W30.00001 Nanotube Radio, KENNETH JENSEN, JEFF WELDON, HENRY GARCIA, ALEX ZETTL, University of California at Berkeley — We have constructed a fully functional, fully integrated radio receiver from a single carbon nanotube. The nanotube serves simultaneously as all essential components of a radio: antenna, tunable band-pass filter, amplifier, and demodulator. A direct current voltage source, as supplied by a battery, powers the radio. Using carrier waves in the commercially relevant 40-400 MHz range and both frequency and amplitude modulation techniques, we demonstrate successful music and voice reception.

2:42PM W30.00002 Template-Based Electroless deposition and TEM Analysis of TiO$_2$ nanotubes¹, ISABEL SCHULTZ, HAIDONG LIU, ZUXIN YE, WENHAO WU, Texas A & M University — We report on the fabrication of TiO$_2$ nanotubes using a template-based electroless deposition method. We used anodic aluminum oxide membranes of pore diameter $\sim$ 200 nm as the templates. The TiO$_2$ nanotubes were fabricated by first dipping the membranes into a titanium tetrafluoride solution at 60 °C for 30 minutes, and then annealing at 225 °C for 2 hours. The composition of the nanotubes verified using the energy dispersive spectroscopy. We used scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to study the surface morphology of the nanotubes extracted after the membranes were dissolved. The nanotubes were found to be uniform along the length of the nanotube. For TEM analysis, an ion-milling technique was also used to produce a thin sample region so that the cross-section of the nanotubes remaining in their original pore channels could be directly imaged. The thickness of the TiO$_2$ nanotubes is about 50 nanometers, and could be controlled by varying the deposition time. Potential applications of these semiconducting TiO$_2$ nanotubes for forming nanostructured semiconducting interfaces will be discussed.

¹Supported by NSF under Grant Nos. DMR-0551813 and DMR-0606529 and DOE under Grant No. DE-FG02-07ER46450

2:54PM W30.00003 Electron Microscopy Analyses of Nanowires Electrochemically Deposited into Porous Membranes¹, HAIDONG LIU, ZHIPING LUO, ZUXIN YE, WENHAO WU, Texas A & M University — We fabricated single crystal nanowires of Zn, Sn and Pb by electrochemically depositing materials into the pores of porous anodic aluminum oxide membranes and polycarbonate membranes. We applied an in situ self-contacting technique to electrically contact single nanowires with macroscopic electrodes of Au, Sn, and Pb pre-fabricated on the membrane surfaces. We observed an anomalous long-range proximity effect in this nanowire/electrode system. In this talk, we describe electron microscopy methods we used to analyze the structure and the composition of the nanowires/electrode system. These included analyses of extracted nanowires using the scanning electron microscope (SEM) and transmission electron microscope (TEM). Nanowires remaining in their original pore channels were also analyzed with TEM using samples prepared by ion-milling and ultramicrotomy. These analyses revealed that the nanowires were single crystalline. Furthermore, the interface between the nanowires and the electrodes were directly imaged. The chemical compositions of the nanowires were also confirmed by the energy dispersive spectroscopy (EDS) analyses and mappings.

¹This work is supported by NSF under Grant Nos. DMR-0551813 and DMR-0606529

3:06PM W30.00004 Characterization of individual SnO$_2$ nanowires with surface science techniques, KAHIBULAKH KATSIEV, ULRIKE DIBOLD, Tulane University, ANDREI KOLMAKOV, Southern Illinois University — Tin oxide is widely used as a solid-state gas sensor for detection of combustible and toxic gases. Recently, the use of nanobelts and nanoribbons has been suggested as novel materials for gas sensing applications. Large-surface-to-volume ratio of the semiconducting metal oxide nanobelts and the congruence of the carrier screening length with their lateral dimensions make them highly sensitive and efficient transducers of surface chemical processes into electrical signal. The surface morphology of an individual nanobelt (NB) was studied with STM. Atomically resolved STM images of NBs reveal an 1X1 (101) SnO$_2$ structure on the top surface of the NB. The thermal stability of the NBs was studied with SEM. The critical temperatures were determined, where structural changes occur in UHV, O$_2$, and air. XPS was used to characterize chemical composition and monitor the cleanliness of the NB material. Ca and C contamination was detected on as-grown SnO$_2$ nanobelts. O plasma, ozone treatment, and annealing in oxygen were used to remove the contaminants.

3:18PM W30.00005 Structure and Stability of Metal Oxide Nanowires, DE NYAGO TAFEN, JAMES LEWIS, West Virginia University, Morgantown, WV — We present a comprehensive theoretical study — within the framework of ab initio density functional theory method — of the structural and stability properties of metal oxide nanowires. We consider nanowires with (100) growth direction with several diameters and surface facet configurations. A stability analysis of the results obtained for these nanowires is used to determine the most stable geometries. We show that the perimeter of the nanowires is a meaningful dimensional parameter, and that the surface facets play a central role on the energetics of the nanowires. The results are compared to available experimental data.
3:30PM W30.00006 First principles investigation of InN non-polar surfaces and nanowires\textsuperscript{1}, ALEKSANDRS TERENCEJEVS, Politecnico of Torino, Torino, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy, GIANGAROLO CICERO, Politecnico of Torino, Torino, Italy — In the last years InN nanostructures have been proposed for application in solar cells, because of the outstanding electronic properties of this nitride compound. An increase of solar energy conversion in these kinds of cells requires a deep knowledge of surfaces properties, and on the effect of confinement on the electronic properties of the material. Here we present an investigation of the structural and electronic properties of InN nanowires as obtained by means of ab initio Density Functional calculations. First we discuss the results for the clean (1-100) and (11-20) faces, which are usually exposed in nanostructures, then we show how InN electronic properties change in nanowires due to confinement effects. We will finally present a possible InN functionalization pathway based on the use of molecules containing thiol groups. Our results show that thiol groups may attach to the surface following an exothermic process (dissociation energy is about 2.5 eV/mol for the (11-20) surface), thus they represent an effective anchoring group for the realization of hybrid InN based devices.

\textsuperscript{1}This work was supported, within the EU FP6, by the ERANET project “NanoSci-ERA: NanoScience in the European Research Area”

3:42PM W30.00007 Van Der Waals Interaction between Two Parallel Radially Deformed Single Wall Carbon Nanotubes\textsuperscript{1}, ADRIAN POPESCU, LILIA WOODS, University of South Florida, IGOR BONDAREV, North Carolina Central University — The van der Waals potential energy is calculated between two parallel infinitely long radially deformed single walled carbon nanotubes within the pairwise Lennard-Jones approximation for extended systems. The nanotubes will undergo different geometrical radial shape transitions if an external hydrostatic pressure with an increasing strength is applied. We describe these shapes with analytically in order to facilitate the calculations. The most preferred mutual orientations are determined in all considered cases in terms of their potential well depths, equilibrium distances, and geometrical parameters. We find that the interaction evolves in such a way as to keep the distance between the interacting surfaces comparable to the graphene-graphene distance in graphite. In addition, the universal graphical potential concept is extended to radially deformed carbon nanotubes. These results can be used as a guide for future experiments to investigate interactions between deformed carbon nanotubes.

\textsuperscript{1}Supported by DOE (DE-FG02-06ER46297).

3:54PM W30.00008 Atomic Structure of the Si(111)-4x1-In System\textsuperscript{1}, BARRY HAYCOCK, West Virginia University & Dublin Institute of Technology, J.D. O’MAHONY, Dublin Institute of Technology — The indium-induced 4 x 1 reconstruction on silicon (111) has been extensively studied due to its unique physical and structural properties, which indicate so-called “Quantum Wire Behaviour”. The likely crystallographic structure of this system has been hotly debated since 1999. The structure was mathematically modeled by Tsay using a planewave calculation method in 2005, which yielded results of atomic positions that matched closely to the Bunk model. In this study we model the th this system using the molecular dynamics (MD) package Fireball, taking as a starting point the atomic positions of the Bunk model. This ab-initio tight-binding MD method has the advantage of being able to operate with a very large number of atoms per cell in a single calculation, thus allowing for a very large superslab in the calculation model. This allows for greater surface area and thus is expected to produce a more accurate surface characteristic calculation result. The results of this calculation are compared to the recent results of Tsay.

\textsuperscript{1}This research is funded by the Irish Research Council for Science Education and Technology.

4:06PM W30.00009 Vapor-solid-solid growth mechanism driven by epitaxial match between solid AuZn alloy catalyst particle and ZnO nanowire at low temperature, RODRIGO LACERDA, LEONARDO CAMPOS, MATTEO TONEZZER, ANDRE FERLAUTO, ROGERIO PANIAGO, SERGIO OLIVEIRA, LUIZ ORLANDO LADEIRA, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, VINCENTZO GRILLO, TASC-INFM-CNR National Laboratory, Trieste, Italy — The present paper provides a comprehensive picture of the precise mechanism of ZnO vapor-solid-solid nanowire growth at low temperatures and gives the fundamental reasons responsible [1]. We demonstrate by using a combination of synchrotron XRD and high resolution TEM that the growth dynamics at low temperatures is not governed by the well-known VLS mechanisms. Based on the Au-Zn phase diagram, temperature measurement and temperature size effects, we show that growth occurs via VSS. The precise composition of the Au-Zn catalyst nanoparticle has been determined to be γ-AuZn. Furthermore, we experimentally observe that there is an indication of a epitaxial relationship between the ZnO nanowires and the γ-AuZn seed particle. A critical new insight on the driving factor of VSS growth is proposed in which the VSS process occurs by a solid diffusion mechanism that is driven by a preferential oxidation process of the Zn inside the alloy catalyst induced by an epitaxial match between the ZnO(10-10) plane and the γ-AuZn(222) plane. [1] L. C. Campos et al, Adv. Materials (accepted for publication).

4:18PM W30.00010 Temperature effects in the stability of pure and doped gold nanowires, ANTONIO J.R. DA SILVA, Instituto de Fisica - USP Brazil, EDWIN HOBIR JR., ADALBERTO FAZZIO, Instituto de Fisica - USP Brazil — Gold nanowires have attracted a great deal of attention, one of the reasons being the ability to form linear gold chains that are one atom wide and that have just a few atoms in length. One of the amazing characteristics of these wires is their stability, even at ambient temperatures. Therefore, it is very important to understand why they are stable and why they break. Moreover, inserted impurities, such as H and C, can dramatically affect their stability. In the present work we use state-of-the-art ab initio molecular dynamics to perform simulations of pure and doped Au nanowires. We propose a general mechanism that helps to explain the stability of these wires and the rupture process. We show that triplets of Au atoms in the neck of atomically thin nanowires have an instability towards rupture at a length of around 6.0-6.1 angstroms. At this length, the potential energy surface (PES) describing the motion of the central atom changes from a single minimum at the middle of the triplet, to a double minimum profile. This provides a consistent picture of the mechanism of rupture of metallic nanowires. Impurities such as C and H also have this behavior. However, as they have stiffer bonds, these PES instabilities always happen in pure Au bonds.

4:30PM W30.00011 Surface Effects on the Electronic, Magnetic and Structural Properties of Free-standing InP nanowires, TOME SCHMIDT, Universidade Federal de Uberlândia — Nanowires due to their large surface-to-volume ratio of particular interest is the understanding of the surface structure and the electronic effects due to surface states. In this work we investigate the structural and electronic properties of InP nanowires aligned along the [111] direction, in which the surface have been studied by passivating with hydrogens or OH radicals and also oxidized. The magnetic properties of Mn doped InP nanowires with different surface termination have been also investigated. Our ab initio density functional calculations show that hydrogen passivation removes the surface states, opening up the band gap. Our results for oxygen adsorbed on the hydrogen passivated InP nanowires, show that there are many configurations where the oxygenes are chemisorbed processes. For Mn doped InP nanowires our results reveal that the surface of the nanocrystals play a fundamental role on the impurity stability and on the magnetic properties of InP nanowires. The formation energy of pairs of Mn impurities in unpasivated nanowires are lower that than of the bulk InP. Most of the Mn pair configurations present FM coupling and their prefer to be inside the nanowire and not on the surface.
4:42PM W30.00012 Shift- and injection-current optical response of BN nanotubes1. NORBERTO ARZATE, Centro de Investigaciones en Optica, Mexico, FRED NASTOS, Department of Physics, University of Toronto, RAUL A. VAZQUEZ-NAVA, Centro de Investigaciones en Optica, Mexico, MIGUEL GONZALEZ, Centro Universitario de los Lagos, Mexico, BERNARDO MENDOZA, Centro de Investigaciones en Optica, Mexico, JOHN SIPE, Department of Physics, University of Toronto — We present the frequency dependence of the electrical shift and injection currents optically generated on BN nanotubes. The shift and injection currents are a second order effect that is associated to a divergence of the nonlinear susceptibility at zero frequency. The shift current is generated with linearly polarized light and the injection current can be generated with circularly polarized light. We make use of density functional theory and pseudopotentials to calculate the nanotube structures and their electronic states. The current-coefficient calculations are done in optical rectification, within the independent particle approximation and within a full band structure scheme. We also obtain the frequency dependence for the shift distance that the center of electron charge moves in the shift-current process and for the swarm velocity or maximum velocity acquired by the electrons in the injection process.

1This work has been partly supported by CONACYT, Mexico, grants: SEP-2004-C01-48142 and SEP-2003-C02-42576.

4:54PM W30.00013 An ab initio study of the interaction of transition metal atoms with single-wall armchair SiC nanotubes1. KAZI ALAM, ASOK RAY — A systematic study of Fe atom encapsulated and adsorbed in armchair SiC nanotubes has been performed using hybrid density functional theory calculations within finite cluster approximation. A detailed comparison of the binding energies, equilibrium positions, Mulliken charges and spin magnetic moments of Fe atoms has been performed for three types of nanotubes. The electronic states, HOMO-LUMO gaps, and changes in gaps with respect to the bare nanotube gaps have been investigated as well. Binding energies of the encapsulated and adsorbed Fe atoms indicate that these structures are stable and show site dependence. For both cases significant band gap decrease is observed for type 1 nanotubes enabling band gap tailoring. This decrease is not observed for the other two types in both cases of interactions. All the structures are found to have magnetic ground states with very high magnetic moments indicating the possibility of them being used as nanomagnets.

1This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

5:06PM W30.00014 Energetics of Cu Nanowires1. MINE KONUK, Department of Physics, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey, BERK ONAT, Informatics Institute, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey, SONDAN DURUKANOGLU, Department of Physics, Istanbul Technical University, Maslak, 34469 Istanbul, Turkey — We have calculated activation energies for several single atom and vacancy diffusion mechanisms on the <100> and <110> axially oriented, rectangular Cu nanowires with a particular interest in determining the effect of varying cross-sectional area on the activation barriers for the investigated processes. The calculations are performed using the nudged elastic band technique based on the interaction potential obtained from the embedded atom method. Our results on activation barriers for adatom diffusion mechanisms indicate a clear dependence on the cross-sectional area of the nanowires. We, furthermore, find that the energy barrier for single vacancy diffusion is decreasing drastically near the outer wall compared to barriers for single vacancy diffusions taking place in the interior region of the nanowire.

1This work is partially supported by TUBITAK under Grant No. TBAG-106T567

5:18PM W30.00015 Ab Initio Computational Studies of the Electronic and Optical Properties of SiC Nanotubes. GUANG-YU GUO, I-JEN WU, Department of Physics, National Taiwan University, Taipei 106, Taiwan — Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima, carbon and other nanotubes have attracted considerable interest worldwide because of their unusual properties and also great potentials for technological applications. Though CNTs continue to attract great interest, other nanotubes such as BN nanotubes (BN-NTs) may offer different opportunities that CNTs cannot provide. We have carried out systematic computational studies of various physical properties of SiC nanotubes. In this talk, we will present ab initio calculations of electronic, linear and nonlinear optical properties of SiC nanotubes [1].


Thursday, March 13, 2008 2:30PM - 5:30PM —
Session W31 DMP GMAG: Focus Session: New Materials and Properties of Complex Oxides
Morial Convention Center 223

2:30PM W31.00001 Magnetic and Structural Properties of Sr-Doped Ba$_2$-$x$Sr$_x$CoO$_4$. HAO SHA, JIANDI ZHANG, Department of Physics, Florida International University, Miami, FL 33199, Q. HUANG, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, Y.O. GARLEA, B.C. SALES, D. MANDRUS, R. JIN, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — We have studied the structural and magnetic properties of a newly synthesized compound Ba$_2$-$x$Sr$_x$CoO$_4$ with different doping ($x$) levels. Monoclinic Ba$_2$CoO$_4$ is an antiferromagnetic (AFM) insulator with Neel temperature $T_N = 25$ K and a two-dimensional character with spins aligned in the ac plane. The isovalent Sr doping causes changes in both crystal structure and magnetic properties. With increasing $x$, $T_N$ initially increases then decreases after reaching the maximum at $x=0.5$. Correspondingly, its crystal structure changes from monoclinic ($x < 0.5$) to orthorhombic ($x \geq 0.5$) at room temperature. The correlation between crystal structure and physical properties will be discussed.

1Supported by NSF-DMR0346826, and DOE DE-FG02-04ER46125

2:42PM W31.00002 Electronic structure changes in novel $J_{eff}$=1/2 system: Ruddlesden-Popper series Sr$_{n+1}$Ir$_n$O$_{3n+1}$ (n=1, 2, and $\infty$). S.J. MOON, J.S. LEE, W.S. CHOI, T.W. NOH, ReCOE & FPRD, Department of Physics and Astronomy, Seoul National University, Korea, H. JIN, J. YU, CSCMR & FPRD, Department of Physics and Astronomy, Seoul National University, Korea, Y.S. LEE, Department of Physics, Soongsil University, Seoul, Korea, V. DURAIARAJ, G. CAO, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA, A. SUMI, H. FUNAKUBO, Department of Innovative and Engineered Materials, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology, Japan — We investigated the electronic structures of Ruddlesden-Popper series Sr$_{n+1}$Ir$_n$O$_{3n+1}$ (n=1, 2, and $\infty$) compounds with optical spectroscopy and first-principles calculation. Among Sr$_{n+1}$Ir$_n$O$_{3n+1}$, while SrIrO$_3$ is a metal, Sr$_2$IrO$_4$ and Sr$_3$Ir$_2$O$_7$ are insulators. In optical conductivity spectra $\sigma(\omega)$, we found unique bandwidth-driven changes of the electronic structures which were quite different from those of 3$d^5$ 4$d^1$ $S=1/2$ systems. From the comparison between $\sigma(\omega)$ and the results of first-principles calculation, we found that the intriguing changes of the electronic structures can be realized by the cooperative interaction between the $S=1/2$ and the electron correlation. These results clearly demonstrate that Sr$_{n+1}$Ir$_n$O$_{3n+1}$ should be considered as a $J_{eff}=1/2$ single band system.

1Supported by NSF-DMR0346826, and DOE DE-FG02-04ER46125
2:54PM W31.00003 Electrical Resistance of Quasi-1D Li$_{0.9}$Mo$_6$O$_{17}$ at Very High Magnetic Field$^1$, CARLOS A.M. DOS SANTOS, Escola de Engenharia de Lorena – USP, J. MORENO, NAMS, The Richard Stockton College of New Jersey, B.D. WHITE, J.J. NEUMEIER, Montana State University, L. BALICAS, NHMFL-Tallahassee — Recently, photoemission experiments, band structure calculations, tunneling, and the description of the electrical resistivity by two power-law terms suggest that Li$_{0.9}$Mo$_6$O$_{17}$ is an excellent example of a metallic Luttinger-liquid (LL) [a,b]. The crossover from metallic to insulating-like behavior near $T_M = 28$ K was addressed by thermal expansion experiments which suggest that a dimensional crossover sets the stage for superconductivity [b]. To obtain more information about the crossover at $T_M$, magnetoresistance measurements were performed under very high magnetic field ($0 < H < 23$ tesla). The results show that the minimum at $T_M$ increases with increasing $H$. The power-law temperature dependence of the electrical resistance at $T_M(H)$ is also evaluated. [a] C. A. M. dos Santos, M. S. da Luz, Yi-Kuo Yu, J. J. Neumeier, J. Moreno, and B. D. White. Submitted to Phys. Rev. Lett. (2007). [b] C. A. M. dos Santos, B. D. White, Yi-Kuo Yu, J. J. Neumeier, and J. A. Souza, Phys. Rev. Lett. 98, 266405 (2007).

$^1$This work was supported by NSF (DMR-0504769 and DMR-0552458) and CAPES (046/05-0).

3:06PM W31.00004 Unconventional magneto-transport in novel layered cobalt oxides, ICHIRO TERASAKI, Waseda University — Among strongly correlated transition-metal oxides, cobalt oxides are known to have unique features arising from the spin-state degree of freedom tightly coupled with Co valence. The Co$^{4+}$ ion in the low-spin state is responsible for anomalous metallic states such as large thermopower in Na$_2$CoO$_3$ and unconventional superconductivity in hydrated Na$_2$CoO$_2$. The Co$^{2+}$ ion favors the high-spin state, which makes magnetic insulators. The Co$^{3+}$ ion is most interesting in the sense that the low-, intermediate- and high-spin states are nearly degenerate, where a spin-state crossover/transition occurs with temperature or pressure. Recently we have discovered two complex layered cobalt oxides, which exhibit unprecedented transport originated from interplay between charge, orbital and spin-states. The first one is Sr$_2$CoO$_{2+}$, in which the Co-O Kagome lattice and two-types of Co-O pillars are stacked along the c axis [1]. The conduction electrons in the Kagome lattice interact with Ising spins in the pillars, and shows two-step plateau in the magnetoresistance along the c axis. The second one is Sr$_2$YCo$_{10}$O$_{25}$, which exhibits a ferromagnetic insulating state below 340 K. Various substitutions of Sr, Y and Co sites dramatically suppress this ferromagnetic state, and concomitantly modify the magneto- and thermoelectric transport. We will discuss the structure-property relationship based on structure analyses. The main part of this work was done in collaboration with S. Ishiwata, W. Kobayashi, and M. Takano.


3:42PM W31.00005 Search for Half-Metallic Antiferromagnetism in Double Perovskites, V. PARDO, University of California Davis, W. E. PICKETT, University of California Davis — The wide class of double perovskite oxides was proposed earlier (PRB 57, 10613 [1998]) as promising for producing a half-metallic antiferromagnet [HMAFM] (more correctly, a spin-compensated half metal). Here we present examples of the affects of structural distortions on the electronic and magnetic properties in selected members. For La$_2$CrNiO$_6$, the idealized perovskite structure had led to a spin-antiparallel state with net moment of 0.6 $\mu_B$, but a ferromagnetic half-metallic state (4 $\mu_B$) was 150 meV per metal atom lower in energy (within local density approximation). Starting with experimental information on LaCoO$_3$ and LaNiO$_3$ and their alloys, we have relaxed the volume and the (seven) internal coordinates within the orthorhombic Pnma space group. The charge states can be characterized by Cr$^{4+}$ and Ni$^{2+}$. The ferromagnetic state is lower by 50 meV within the generalized gradient approximation. Using LDA+U ($U=3$ eV on each transition metal ion) opens a gap of 0.6 eV (FM insulator) and is favored by 120 meV over the antialigned state. Although no HMAFM state is obtained, these results show that structural relaxation must be suppressed this ferromagnetic state, and concomitantly modify the magneto- and thermoelectric transport. We will discuss the structure-property relationship based on structure analyses. The main part of this work was done in collaboration with S. Ishiwata, W. Kobayashi, and M. Takano.


3:54PM W31.00006 Electrical transport and thermodynamic properties of SrNbO$_{3.41}$, ARIANA DE CAMPOS, Montana State University, ANN DEML, University of Wisconsin-River Falls, B.D. WHITE, Montana State University, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena-USP, M.S. DA LUZ, J.J. NEUMEIER, Montana State University — In 1991, Lichtenberg et al.$^1$ reported the electric conductivity of SrNbO$_{3.41}$ revealing quasi-1D behavior. This system offers many possibilities to vary the compositional, structural, chemical, and physical properties.$^1$ Depending upon the temperature range and crystallographic direction, it exhibits metallic behavior or a metal-semiconductor transition. In this work, the properties of SrNbO$_{3.41}$: single crystals are revisited. The single crystals were grown by the floating zone method and characterized by x-ray diffraction. Electrical resistivity as a function of temperature was measured with four-probe and Montgomery methods. We will also report results of heat capacity and thermal expansion measurements.$^2$ F. Lichtenberg et al., Z. Phys. B 84, 369 (1991); F. Lichtenberg et al., Prog. Solid State Chem 29, 1-70 (2001).

$^1$This material is based upon work supported by the Brazilian Agency CNPq (Grant No. 201439/2007-7), the NSF (Grant No. DMR-0504769) and U.S. DOE Office of Basic Energy Sciences (Grant No. DE-FG-06ER46269).

4:06PM W31.00007 Extreme electron-phonon coupling in magnetic rubidium sesquioxide, ROBERT DE GROOT, Rijksuniversiteit Groningen, JISK ATTEMA, Radboud University, S. RIYADI, GREÃŒME BLAKE, Rijksuniversiteit Groningen, GILLES DE WIJS, Radboud University, THOMAS PALSTRA, Rijksuniversiteit Groningen — Rb$_2$O$_3$ is a black, opaque oxide. Early work suggests that the stability range of the sesquioxide phase in the rubidium-oxygen phase diagram is rather broad. Rb$_2$O$_3$ remains cubic down to the lowest temperature measured (5 K). The open oxygen form dumbbells with interatomic distances in between those of peroxide and superoxide anions, and strong athermal motion persists down to low temperatures. [1] Electronic-structure calculations show that the dynamics at low temperature is caused by 6 phonon modes of zero frequency, which induce a very strong electron-phonon interaction. The softness of half of these modes is suppressed by the application of pressure. Calculated using the average oxygen positions, rubidium sesquioxide is a half-metallic ferromagnet. [2]

[1] CR CHIM (11-13); 591-594 NOV 1999

4:18PM W31.00008 Gigantic optical magneto-electric effect in CuB$_2$O$_4$, MITSURU SAITO, KOUJI TANIGUCHI, TAKAHISA ARIMA, Tohoku University — It has been recognized since 1960s that magneto-electric (ME) materials may also show an optical magneto-electric (OME) effect showing up as a change in optical absorption with reversal of the propagating direction of light. The OME effect is an interesting object of scientific research and provides possibilities for applications. However, the changes in absorption coefficient ever discovered were very small (less than 0.2%). We present a gigantic OME effect in a noncentrosymmetrical weak ferromagnet CuB$_2$O$_4$, in which the absorption coefficient changes by a factor of three with reversal of a very weak magnetic field of 300 eC. This magnitude of OME effect enables us to observe it by a CCD camera with linearly polarized near-infrared and visible light. Spectroscopic study and comparison of OME effect with magnetization indicate an important role of canted antiferromagnetic spin ordering and local symmetry of a square Cu$^{2+}$ site. The gigantic OME effect can be applicable to optical devices like magnetic switching of color in the future.
4:30PM W31.00009 Resonant inelastic X-ray scattering study of quasi-zero-dimensional copper metaborate. JASON HANCEOK, GUILLAUME CHABOT-COUTURE, MARTIN GREVEN, Stanford University, GUERMAN PETRAKOVSKI, Kirenskii Institute, Siberia, KENJI ISHII, JUN'ICHIRO MIZUKI, Japan Atomic Energy Agency — Cu$_2$O$_6$ consists of many CuO$_6$ plaquettes separated by B ions. We report a study of the electronic excitation spectra of this system in order to explore the relationship between excitation symmetry and the resonant inelastic X-ray scattering (RIXS) technique. We find a small number of well separated features in the experimentally accessible range of 0.5-15 eV energy transfer, and weak dispersion is suggestive of the quasi-zero-dimensional nature of this system. Systematic trends in the data are suggestive of a composite nature to one of the observed features. Using a cluster model, we describe these unexpected trends and clarify how the choice of experimental geometry selectively influences the sensitivity to particular excitation symmetries in the RIXS experimental technique.

4:42PM W31.00010 Powder neutron diffraction study of quasi-one-dimensional Li$_0.9$Mo$_6$O$_{17}$

MARIO S. DA LUZ, Montana State University, C.A.M. DOS SANTOS, Escola de Engenharia de Lorena, B.D. WHITE, J.J. NEUMEIER, Montana State University, Q. HUANG, J.B. LEAO, J.W. LYNN, NIST Center for Neutron Research — The crystallographic structure of quasi-one-dimensional Li$_0$$_9$Mo$_6$O$_{17}$ was investigated by Rietveld refinement of powder neutron diffraction data at temperatures in the range 5 K < T < 295 K. Structural parameters, atomic positions, occupation numbers, and isotropic thermal parameter B$_{iso}$ will be reported. The occupancy was refined revealing a Li occupancy greater than 0.9. Bond valences sums will also be reported for various Li and Mo sites. At room temperature, the crystal was found to exhibit monoclinic symmetry with space group P21/c and lattice parameters $a = 12.7506(1)$, $b = 5.5242(1)$, $c = 9.4913(2)$ and $\beta = 90.593(1)^\circ$. Good agreement between the temperature dependence of lattice parameters and high resolution thermal expansion results was obtained. *C. A. M. dos Santos, B. D. White, Yi-Kuo Yu, J. J. Neumeier, and J.A. Souza, Phys. Rev. Lett. 98, 266405 (2007).*

5:06PM W31.00012 X-ray absorption and x-ray magnetic dichroism study on Ca$_3$CoRhO$_6$ and Ca$_2$FeRh$_2$O$_6$. TOBIAS BURNUS, ZHIWEI HU, University of Cologne, Germany, JULIO C. CEZAR, European Synchrotron Radiation Facility, Grenoble, France, SEIJI NITAKA, KENJI ISHII, JUN'ICHIRO MIZUKI, Japan Atomic Energy Agency — We have investigated the structural and physical properties of Ca$_3$CoRhO$_6$ single crystals using x-ray absorption and x-ray magnetic dichroism. The magnetic susceptibility data indicate that there are several magnetic transitions above room temperature. The possible correlation between charge, spin, and lattice will be explored.

5:18PM W31.00013 Anisotropy in magnetic properties of single crystal LiFePO$_4$. GAN LIANG, Sam Houston State University, KEESONG PARK, JOHN MARKERT, University of Texas at Austin, JIYING LIAO, DAVID VANKIN, Ames Lab and Iowa State University — We report the experimental and theoretical results on the anisotropies in the magnetic properties and x-ray absorption spectra of single crystal LiFePO$_4$. A mean-field theory is developed to explain the observed strong anisotropies in Lande g-factor, paramagnetic Curie temperature, and effective moment for LiFePO$_4$ single crystals. The values of the in-plane nearest- and next-nearest-neighbor spin-exchange ($J_1$ and $J_2$), inter-plane spin-exchange ($J_3$), and single-ion anisotropy ($D$), obtained recently from neutron scattering measurements, are used for calculating the Curie temperatures with the formulas derived from the mean-field Hamiltonian. It is found that the calculated Curie temperatures match well with that obtained by fitting the magnetic susceptibility curves to the modified Curie-Weiss law.

Thursday, March 13, 2008 2:30PM - 5:30PM —

Session W32 GMAG DMP FIAP: Focus Session: Domain Wall Motion and Itinerant Magnetism

2:30PM W32.00001 Domain wall motion under the non-uniform transverse magnetic field with rigid domain structure. CHUN-YEOL YO, Dept. of Phys. Inha University — Another method for the domain wall movement in a nanowire geometry with rigid domain structure will be proposed. We find that a transverse domain wall move to the energy minimum position under a non-uniform transverse magnetic field in order to minimize the Zeeman energy. By the collective coordinate approach, the domain wall dynamics under non-uniform transverse magnetic field in nanowire geometry is investigated. The validity of concept of the present method and the domain wall equation of motion are confirmed by micromagnetic simulations. It is found that the domain wall velocity of a few 100 m/s can be obtained for the moderate conditions based on the analytic and numerical studies. The direction of the domain wall movement depends only on the magnetization direction inside of the domain wall itself, not on the one of the domain. Therefore, it is possible to achieve field driven domain wall motion with rigid domain structures. The non-uniform transverse magnetic field driven domain wall motion has a superior nature of the rigidity of the domain structure during the domain walls movement in addition to the all advantages of conventional field driven domain wall movement.
2:42PM W32.00002 Crossed Ratchet Effects for Magnetic Domain Wall Motion1, JOSE I. MARTIN, A. PEREZ-JUNQUER, Dpto. Fisica, U. Oviedo, Spain, V.I. MARCONI, A.B. KOLTON, Dpto. Fisica Atomica Molecular y Nuclear and GISC, U. Complutense, Madrid, Spain, L.M. ALVAREZ-PRADO, Dpto. Fisica, U. Oviedo, Spain, Y. SOUCHE, Inst. Neel, CNRS and U. Joseph Fourier, Grenoble, France, A. ALIJJA, M. VELEZ, Dpto. Fisica, U. Oviedo, Spain, J.V. ANGIUTA, IMMM, CNM, CSIC, Tres Cantos, Spain, J.M. ALAMEDA, Dpto. Fisica, U. Oviedo, Spain, J.M.R. PARRONDO, Dpto. Fisica Atomica Molecular y Nuclear and GISC, U. Complutense, Madrid, Spain — The driven motion of domain walls in extended amorphous magnetic films patterned with a periodic array of asymmetric holes has been studied experimentally and theoretically. We find two crossed ratchet effects of opposite sign that change the preferred sense for domain wall propagation, depending on whether a flat or a kinked wall is moving. These crossed effects have an interesting consequence with potential applications: the system keeps memory of the sign of the last saturating state even in a zero magnetization configuration. By solving numerically a simple $\phi^4$-model we show that the essential physical ingredients for this effect, the competition between drive, elasticity and asymmetric pinning, are quite generic and could be realized in other experimental systems involving elastic interfaces moving in multidimensional ratchet potentials.

1Work Supported by Spanish CICYT (NAN2004-09087, MOSAIKO, and FIS2005-07392)

2:54PM W32.00003 In Situ TEM Observation of Current-Induced Domain Wall Motion in Patterned Permalloy Wires1, TODD BRINTLINGER2, JOHN CUMINGS3, University of Maryland — Using a transmission electron microscope (TEM) operating in Lorentz mode, we observe the movement of a domain-wall due to the flow of current in a permalloy wire. The wire is formed on electron-transparent silicon nitride membranes using standard electron beam lithography and thermal vacuum deposition. The resulting wire geometry is 30 nm thick, ~100nm wide, and microns long. A custom-built electrical measurement stage and palladium leads deposited on top of the permalloy wires allow in situ measurements on the wire in the TEM. Lorentz mode imaging (Fresnel contrast) allows the determination of the domain wall location. We observe the domain wall to move in the direction of electron flow, with a current density of around $1 \times 10^{11}$ A/m$^2$ being required to move the wall. We will present the nanofabrication process, results, and interpretation of these experiments.

1This work was supported by NSF MRSEC DMR 0520471 and conducted at the Maryland Nanocenter. We acknowledge the use of the NISP laboratory, a MRSEC shared equipment facility.
2Dept of Materials Science and Eng.
3Dept of Materials Science and Eng.

3:06PM W32.00004 Stochastic Current-Driven Domain-Wall Motion Observed by X-Ray Microscopy, GUIDO MEIER, University of Hamburg, Germany — Transmission x-ray microscopy can directly visualize the influence of a spin-polarized current on the magnetization of micro- and nanostructures. We investigate the stochastic motion of domain walls in curved wires [1] and the motion of vortices in squares [2]. To observe domain-wall motion pulses of nanosecond duration and high current density are send through permalloy wires and either move or deform the domain wall. The current pulses have nanosecond duration and a high current density of up to $1.0 \times 10^{12}$ A/m$^2$ and drive the wall either undisturbed, i.e. as a composite particle through the wire or causes structural changes of the magnetization. Repetitive pulse measurements reveal the stochastic nature of current induced domain-wall motion. From the experiments we estimate the ratio between the degree of nonadiabatic and the Gilbert damping parameter indicating the importance of the nonadiabatic contribution to current driven domain-wall motion. To compare experimental results with theory the spin-torque transfer model of Zhang and Li [3] is implemented in the micromagnetic framework OOMMF [4]. The code is applied to determine the current-induced domain wall velocity using the material parameters of permalloy. The simulations support the interpretation of the experimental results. Sinusoidal high-density currents are applied to micrometer-sized permalloy squares containing ferromagnetic vortices. Spin-torque induced vortex gyration on the nanosecond timescale is observed. The phase of the gyration in structures with different chirality are compared to an anamorphic model and micromagnetic simulations, considering both alternating spin-polarized currents and the current’s Oersted fields. This analysis reveals that spin-torque is the main source of motion. Supported by the DFG via SFB 668 and GK 1286 as well as by the U.S. DOE Contract No. DE-AC02-05-CH11231. References:

3:42PM W32.00005 The dynamics of field and current-driven magnetic domain wall depinning1, GEOFFREY BEACH, UT Austin, CARL KNUTSON, MAXIM TSOI, JAMES ERSKINE — The depinning of a magnetic domain wall from a well-defined potential well was studied experimentally on timescales ranging from minutes down to tens of nanoseconds. At longer timescales, the behavior follows the classical Neel-Brown model of thermal activation, one of the few observations of this process for the ideal case of a single energy barrier. Below one microsecond, however, the depinning rate becomes independent of the activation volume and assumes a more universal behavior. This transition is due to a vanishing of the energy barrier at a critical field, beyond which the rate of de pinning depends primarily on the torque supplied by the field and spin current. A dc spin-polarized current flowing across the domain wall has the effect of lowering the energy barrier by an amount that is predominantly quadratic in current, independent of its direction. This is seen to arise from a shift of the wall in the energy potential due to the adiabatic component of spin-transfer torque.

1Supported by NSF-DMR-0404252 and the R. A. Welch Foundation


4:06PM W32.00007 Domain wall motion by subcritical harmonic current, YURY ADAMOV, ARTEM ABANOV, JAIRO SINOVA, Texas A&M University — We consider the behavior of the domain wall in the bianisotropic magnetic wire. We show that while the domain wall cannot be moved by the constant current below the certain threshold value (critical current), if we add an alternating component to the current the domain wall starts to move with nonzero velocity. We obtain the analytic expression for this velocity and make suggestions of possible experiments.
4:18PM W32.00008 Theory of Electromotive Force Induced by Domain Wall Motion, SHENGYUAN YANG, DI XIAO, QIAN NIU, Department of Physics, The University of Texas at Austin — We formulate a theory on the dynamics of conduction electrons in the presence of moving magnetic textures in ferromagnetic materials. We show that the variation of local magnetization in both space and time gives rise to topological fields, which induce electromotive forces on the electrons. Universal results are obtained for the emf induced by both transverse and vortex domain walls traveling in a magnetic film strip, and their measurement may provide clear characterization on the motion of such walls.

4:30PM W32.00009 Oscillatory domain wall motion in a single-crystal ultrathin Au/Co/Au system, KEOKI A. SEU, Physics Department, University of Oregon and Advanced Light Source, Lawrence Berkeley National Laboratory, SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, SUNGYUN PARK, Busan Center, Korea Basic Science Institute, Busan 609-735 Korea, CHARLES M. FALCO, College of Optical Sciences, University of Arizona, STEPHEN D. KEVAN, Physics Department, University of Oregon — We have used x-ray photon correlation spectroscopy together with resonance soft x-ray scattering to measure domain dynamics in a Au/Co/Au system that exhibits a spin reorientation phase transition (SRT) in the temperature range of 200-300 K. The incoming photon energy was tuned at the Co L3 edge and the coherence is established with a ~10 nm pinhole. The resultant speckle pattern is measured with a CCD camera in time as a function of temperature 200 K to 300 K. The correlation coefficient, which is an indicator of domain wall dynamics, shows damped oscillatory behavior in time. The period of the oscillations is approximately 120 sec. The frequency and damping constant were found to depend on the length-scale and temperature changes through the phase transition. Our results show that the SRT dynamics on a mesoscopic length scale and slow time scale can be surprisingly complex.

4:42PM W32.00010 Thermodynamics of Itinerant Magnets: A Simple Classical Model with Longitudinal Spin Fluctuations, JAMES GLASBRENNER, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — The effects of longitudinal spin fluctuations (LSF) on the thermodynamics of magnetic metals are studied using a model Hamiltonian with only one “ityperance parameter.” We performed Monte Carlo simulations and compared the results with the mean-field theory. A non-trivial complication is the choice of phase space measure. We explored two options: the “classical” measure and the “flat” measure. Our central result is that magnetic short-range order is always weak, and the mean-field theory is in a very good agreement with Monte Carlo results. Additionally, the results are very sensitive to the choice of the phase space measure, which is a limitation of our model. Nevertheless LSF are essential for the correct description of magnetic thermodynamics and their absence in the adiabatic approximation leads to unphysical results for itinerant systems. Deviations from the Curie-Weiss law due to LSF are also observed and discussed.

4:54PM W32.00011 High Pressure Study of Magnetic Order in an Itinerant Electron System: Investigating Weak vs. Strong Coupling, RAFAEL JARAMILLO, The University of Chicago, Y. FENG, J. C. LANG, Z. ISLAM, APS, Argonne National Laboratory, T. F. ROSENBAUM, The University of Chicago — We measure directly the spin- and charge-density-wave order parameters of the itinerant antiferromagnet Cr via x-ray diffraction as the system is driven towards its quantum critical point with pressure using diamond anvil cell techniques. The exponential decrease of the spin and charge diffraction intensities with pressure confirms the harmonic scaling of spin and charge in this incommensurate system, while the evolution of the incommensurate ordering vector provides important insight into the difference between tuning with pressure and chemical doping. Measurement of the charge density wave over several orders of magnitude of diffraction intensity provides the clearest demonstration to date of a weakly coupled BCS-like ground state. Evidence for coexistence of this weak coupling ground state with incipient magnetic fluctuations at high temperatures in chromium and other more strongly coupled systems raises intriguing questions about the meaning of weak vs. strong coupling and suggests a new category of quantum phase transitions.

5:06PM W32.00012 Dynamic susceptibility of itinerant ferromagnets in the ordered state1, MATTHEW VANNETTE, SERGEY BUD’KO, PAUL CANFIELD, RUSLAN PROZOROV, Iowa State University, Dept of Physics & Astronomy and Ames Laboratory — Measurements of radio-frequency dynamic susceptibility of ferromagnets exhibit striking differences between local moment and itinerant systems. Whereas local moment systems show a sharp peak at the Curie temperature ($T_c$) which evolves to higher temperatures and lower amplitudes with applied dc magnetic field, itinerant systems show a broad maximum at temperatures well below $T_c$. The itinerant system’s maximum is suppressed in amplitude and shifts to lower temperatures with applied dc magnetic field. Existing Stoner or spin fluctuations theories derive strictly zero-field susceptibility and we propose a generalization of these models to incorporate the effect of applied dc field. A good agreement between our semi-phenomenological approach and experimental results obtained on several generally accepted itinerant materials with various $T_c$’s is presented.

5:18PM W32.00013 Elementary excitations in antiferromagnetic Heisenberg spin segments, MARCO AFFRONTE, CNR-INFM-S3 and University of Modena, ALBERTO GHIRRI, MARCO EVANGELISTI, ANDREA CANDINI, CNR-INFM-S3, STEFANO CARRETTA, PAOLO SANTINI, GIUSEPPE AMORETTI, University of Parma, Dpt of Physics, RACHEL DAVIES, GRIGORE TIMOC, RICHARD WINPENNY, University of Manchester, CNR-INFM-S3 TEAM, UNIVERSITY OF PARMA TEAM, UNIVERSITY OF MANCHESTER TEAM — We report on ac-susceptibility, low temperature magnetization and specific heat measurements on molecular compounds, shortly named (Cr$_2$)$_2$, (Cr$_2$)$_2$, Cr$_3$, (NCCr)$_2$Nz, that comprise different variants of spin arrays. These systems constitute real examples of collections of identical antiferromagnetic Heisenberg spin segments. We indeed show that this picture, with dominant exchange term in the spin Hamiltonian ($J/k_B$ ranging from 13 to 16 K in all compounds) and weak anisotropy term, fits well the measured physical properties. The character of energy spectra of these variants with those of similar cyclic spin systems evidences effects associated to: i) the breaking the cyclic boundary conditions and ii) odd and even nuclearity of spin segments.

Thursday, March 13, 2008 2:30PM - 5:30PM –
Session W33 GMAG FIAP DMP: Focus Session: Spins in Narrow Gap Semiconductors Morial Convention Center 224

2:30PM W33.00001 Spin Injection, Manipulation, and Detection, in InAs Nanodevices1, C.M. JONES, B.T. JONKER, B.R. BENNETT, J.R. MEYER, M.E. TWIGG, T.L. REINECKE, D. PARK, S.V. PEREVERZEV, C.S. BADESCU, C.H. LI, A.T. HANBICKI, O. VAN TERVE, I. VUGRAFTMAN, Naval Research Laboratory — In this talk the authors will discuss their progress using InAs heterostructures to produce spin-polarized injection and detection, as well as manipulation of coherent spin-polarized electrons for a spin-based FET (SpinFET). High-quality n-type InAs heterostructures demonstrate many favorable characteristics necessary to the study of spin dynamics, including 2DEG’s with small effective mass ($m^* = 0.023$) and large g-factor (g = -15). Previously, high-mobility InAs heterostructures have been demonstrated in which electrons pass ballistically over hundreds of nanometers up to room temperature. Our devices seek to exploit the strong Spin-Orbit effect present in InAs to manipulate coherent spin-polarized electrons during transport, by producing perpendicular electric field using isolated top-gates fabricated over the electron transport region.

1This work was supported by ONR.
2:42PM W33.00002 Electrical Spin Injection into InAs Wetting Layer – CONNIE H. LI, GEORGE KIOSEOGLOU, AUBREY T. HANBICKI, RAMASI GOSWAMI, STEVE HELLBERG, BERRY T. JONKER, Naval Research Lab, MESUT Yasar, ATHOS PETROU, SUNY Buffalo — InAs is an attractive material for optoelectronic and high-speed transistor devices due to its large bandgap and high electron mobility. Owing to its large Rashba spin-orbit coupling, the 2DEG formed in InAs-based heterostructures has also been proposed for spin transport within a spin FET. Here we demonstrate efficient spin injection from Fe into a thin (~3ML) InAs wetting layer (WL) that forms on GaAs before the formation of QDs. Cross sectional TEM shows that the WL is continuous laterally over many microns, and transport measurements reveal 2DEG-like behavior. The WL electron magnetic focusing effect is observable up to 150 K, while the multiplet structure in the maxima shows a more pronounced temperature dependence and fades at higher temperature. Our observation is important to understand zero-field spin splitting mechanisms in a system with strong-spin orbit interaction.

Supported by: NSF-DMR-0507866 and AFOSR Young Investigator Program 06NE231.

3:06PM W33.00004 Spin coherence times in n-type InSb thin films – R.L. KALLAHER, J.J. HEREMANS, Department of Physics, Virginia Tech, Blacksburg, VA — In order to investigate the spin coherence times in the narrow gap semiconductor InSb, low temperature magnetoresistance measurements were performed on Te-doped thin films of InSb in weak perpendicularly applied magnetic fields. The measured changes in the resistance, as a function of applied field, in these n-type films show anti-localization phenomena that occur as a consequence of the strong spin-orbit interaction present in InSb. Hence, the magnitude of both the spin and the coherence times of the electrons in InSb can be determined by fitting the measured magnetoresistance curves to a localization theory that includes the effects of spin-orbit scattering. Such fits reveal that for the Te-doping levels investigated, the spin coherence times vary from approximately 20 ps to 200 ps at low temperatures, with very weak or no temperature dependence below 10 K. Furthermore, by analyzing the spin coherence times in films with different Te-doping densities, it is shown that the Elliot-Yafet mechanism is responsible for the spin decoherence in doped InSb at low temperatures.

Supported by: NSF-DMR-0507866 and NSF-DMR-0520550.

3:30PM W33.00006 Temperature dependence of spin-resolved transverse magnetic focusing in InSb- and InAs heterostructures – J.J. HEREMANS, R.L. KALLAHER, R.B. LILLIANFELD, Virginia Tech, HONG CHEN, University of North Florida, N. GOEL, S.J. CHUNG, M.B. SANTOS, University of Oklahoma, W. VAN ROY, G. BORCHARS, IMEC (Belgium) — Spin-orbit interaction in InSb/InAlSb and InSb/AlGaSb heterostructures leads to spin-split orbital motion. The spatial separation of semiclassical cyclotron orbits is experimentally detected by measuring the magnetoresistance of lithographically patterned mesoscopic ballistic transverse magnetic focusing geometries. The 1st and 2nd focusing maxima show multiplet structure, consistent with spin-split ballistic orbits and spin-dependent reflection off the focusing barrier. In InSb, the transverse magnetic focusing effect is observable up to 150 K, while the multiplet structure in the maxima shows a more pronounced temperature dependence and fades by 80 K. In InAs, the transverse magnetic focusing effect persists to 60 K, and the multiplet structure is visible up to 20 K. The difference in temperature dependence between maxima and multiplet structure indicates that a length scale separate from the mean-free-path governs the observation of splitting, pointing to the use of transverse magnetic focusing for quantifying the temperature dependence of spin coherence. (NSF DMR-0618235, DMR-0080054, DMR-0209371)

3:42PM W33.00007 External electric field effects on AAS oscillations in narrow gap semiconductors – R. B. LILLIANFELD, R. L. KALLAHER, D. E. DAVIS, J. J. HEREMANS, Virginia Tech, HONG CHEN, University of North Florida, N. GOEL, S. J. CHUNG, M. B. SANTOS, University of Oklahoma, W. VAN ROY, G. BORCHARS, IMEC (Belgium) — We present experiments on quantum interference phenomena in semiconductors with strong spin-orbit interaction, using mesoscopic parallel ring arrays fabricated on InSb/InAlSb and InAs/AlGaSb heterostructures. From gate modulation, the WL is continuous laterally over many microns, and transport measurements reveal 2DEG-like behavior. The WL low temperature resistance of the ring arrays as a function of weak perpendicularly applied magnetic fields as well as applied gate voltage. The low field magnetoresistance in the arrays has the h/2e periodicity characteristic of Altschuler-Aronov-Spivak (AAS) oscillations. Despite reduced gate action typical of narrow-gap heterostructures (characterized by Hall measurements), we note an effect on the oscillatory magnetoresistance. The AAS oscillation magnitudes acquire a quasi-periodic modulation as function of gate voltage, and the localization background broadens at higher electron densities. The nature of these influences is examined. (NSF DMR-0618235, DMR-0080054, DMR-0209371)

3:54PM W33.00008 Measurements of spin polarization and spin relaxation in 2D electron gases – S.M. FROLOV, University of British Columbia, A. VENKATESAN, W. YU, J.A. FOLK, UBC, W. WEGSHEIDER, University of Regensburg — Pure spin currents are generated and detected using quantum point contacts in narrow channels of a GaAs/AlGaAs 2D electron gas. A spin relaxation length of 50 microns is achieved due to a cancellation of Rashba and Dresselhaus spin-orbit interactions along 110 crystal direction. Spin currents observed at zero magnetic field are correlated with the 0.7 conductance feature of quantum point contacts, suggesting static spontaneous spin polarization.
The spin interference effect was investigated for square and rectangular loop arrays that were nanostructured in InGaAs/InAlAs quantum wells. The Rashba and Dresselhaus terms quantitatively. Koga et al., PRB 70, 161302(R) (2004); ibid. 74, 041302(R) (2006). [2] Koga et al., phys. stat. sol. (C) 3, 4220 (2006).

4:18PM W33.00010 Aharonov-Casher effect in hole ring with spin-orbit interaction, MARIO BORUNDA, ALEXEY KOVALEV, Physics Department, Texas A&M University, TOMAS JUNGWIRTH, Institute of Physics, Academy of Sciences of the Czech Republic, LAURENS MOLKEN, Physikalisches Institut (EP3), Universität Würzburg, JAIRO SINOVA, Physics Department, Texas A&M University — We study the quantum interference effects induced by the Aharonov-Casher phase in a ring structure two-dimensional heavy-hole (HH) system with spin-orbit interaction. The influence of the spin-orbit interaction on the transport causes interference effects which are a signature of the topological Aharonov-Casher phase. We present numerical calculations of the magnetocconductance and spin dependent transport in realistic semiconductor ring structures.

4:30PM W33.00011 Plasmons of a two-dimensional electron gas with Rashba and Dresselhaus spin-orbit coupling, JESUS A MAYTORENA, CATALINA LOPEZ-BASTIDAS, Centro de Ciencias de la Materia Condensada, UNAM Ensenada, Mexico, ELMER CRUZ, CICESE, CCMC UNAM, Ensenada, Mexico — We calculate the dielectric response of a two-dimensional electron gas with both Rashba and Dresselhaus spin-orbit (SO) coupling within the self-consistent-field approach. We obtain the dispersion relations of the collective modes and the regions of single-particle excitations, related with intra- and inter-spin transitions. The interplay of both types of SO couplings give rise to an angular anisotropy of the spin-splitting energy. As consequence, the plasmon spectrum and the Landau damping regions show a dependence on the direction of the wave vector transfer. This response is in contrast to that of vanishing Rashba or Dresselhaus case. We also discuss the dependence of this spectral characteristics on the electron density and SO coupling strengths, and derive expressions for the intra- and inter- SO plasmons in the long-wavelength limit.

4:42PM W33.00012 Magnetoplasmon excitations in Rashba spintronic quantum wires: Maxons, rotons, and negative-B dispersion, MANVIR KUSHWAHA, University of Puebla, Puebla, Mexico — We report on the theoretical investigation of plasmon excitations in a quasi-two-dimensional electron gas in the presence of a harmonic potential, a perpendicular magnetic field, and the spin-orbit interaction (SO) induced by the Rashba effect. The result system is a Q1D quantum wire with free propagation in the y direction and magnetoelectric quantization along the x. The problem involves three length scales: \( l_0 = \sqrt{\hbar/m^*\omega_c} \), \( l_r = \sqrt{\hbar/m^*\omega_r} \), and \( l_d = h^2/(2m^*\alpha) \), which characterize the relative strengths in the interplay of confinement, the magnetic field, and the Rashba SOI. The resulting Schrödinger-like equations are two coupled equations, which cannot be solved in an explicit form. However, invoking the limits of a strong magnetic field, \( l_r \ll l_0 \) and \( l_d \ll 1 \) allow us to solve this set of coupled equations exactly. We then derive and discuss the dispersion relations for collective excitations within the framework of Bohm-Pines’ RPA. The intrasubband and intersubband magnetoplasmons in a Q1DEG are characterized, respectively, by the negative-B dispersion and the magnetoroton excitation. Here we scrutinize the effect of the Rashba SOI on these characteristics in depth. We observe that the SOI modifies drastically the behavior of both magnetoplasmons in the long wavelength limit and may render them relatively more susceptible to the Landau damping in the short wavelength limit.

4:54PM W33.00013 Resonant spin polarization and Hall conductances in a two-dimensional electron gas, DEGANG ZHANG, Texas Center for Superconductivity and Department of Physics, University of Houston, TX 77204, YAO-MING MU, Center for Advanced Materials, University of Houston, TX 77204, CHIN-SEN TING, Texas Center for Superconductivity and Department of Physics, University of Houston, TX 77204 — We have studied transport properties in a two-dimensional electron gas with equal Rashba and Dresselhaus spin-orbit interactions under a perpendicular magnetic field. By employing the exact solution for this system, we found resonant charge and spin Hall conductances at a certain magnetic field, where all the nearest-neighboring Landau levels cross. Near the magnetic field, there exists a resonant spin polarization, which can also induce resonant charge and spin Hall effects.

5:06PM W33.00014 Spin signal recovery in a two-dimensional electron gas with a quantum point contact, JAE-SEUNG JEONG, HYUN-WOO LEE, Department of Physics, Pohang University of Science and Technology — We study transport properties of the spin-polarized current in a two-dimensional electron gas (2DEG) including a quantum point contact (QPC) in the presence of Rashba spin-orbit (RSO) coupling. Spin-resolved conductance is investigated numerically using a recursive Green function method, with special attention to the quantum effects of spin-charge transport channels. It is found that when the conductance is examined as a function of the RSO coupling strength, the conductance modulation ratio, defined as the ratio between the maximum and minimum conductances, can be enhanced by the QPC in the ballistic and weakly diffusive regime as well. Decaying rate of the spin-polarization can be also reduced.

5:18PM W33.00015 Semiclassical Equations of Motion for Bloch Electrons in External Fields, Including Spin-Orbit Interaction, W.C. KERR, Wake Forest U. — This talk considers an electron moving in a periodic potential with spin-orbit interaction and perturbed by external slowly varying electric field and uniform magnetic field. Superposition of the time-independent Bloch spinor states of the unperturbed Hamiltonian gives a wave packet state with both wavevector space and spin-orientation amplitude factors. The time-dependent variational principle produces equations of motion for the wave packet in both configuration and wavevector space and for the spin-orbit orientation factors. For spinless electrons this procedure yields the familiar semiclassical equations of motion augmented by an orbital magnetic moment contribution to the Bloch band energy and an “anomalous velocity” proportional to a Berry curvature. The inclusion of spin-orbit interaction gives additional contributions to the velocity involving different Berry curvatures. One is a spin-dependent contribution to the magnetic moment, and another is an electric dipole-like contribution that is also proportional to the spin operator.

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Thursday, March 13, 2008 2:30PM - 5:30PM — Session W35 FIAP: Focus Session: Nanotechnology II Morial Convention Center 227
2:30PM W35.00001 TEBAL: Nanosculpting devices with electrons in a transmission electron microscope1. MARIJA DRNDIC, University of Pennsylvania — Manipulation of matter on the scale of atoms and molecules is an essential part of realizing the potential that nanotechnology has to offer. In this talk I will describe transmission electron beam ablation lithography (TEBAL), a method for fabricating nanostructures and fully integrated devices on silicon nitride membranes by nanosculpting evaporated metal films with electron beams. TEBAL works by controllably exposing materials to an intense and highly focused beam of 200 keV electrons inside the transmission electron microscope (TEM). The effect of electron irradiation can be used to controllably displace or ablate regions of the metal with resolution on the scale of tens of atoms per period. In situ TEM imaging of the ablation action with atomic resolution allows for real-time feedback control during fabrication. Specific examples presented here include the fabrication and characterization of nanogaps, nanorings, nanowires with tailored shapes and curvatures, and multi-terminal devices with nanoscale gaps between the terminals. These nanostructures are fabricated at precise locations on a chip and seamlessly integrated into large-scale circuitry. I will discuss how the combination of high resolution, geometrical control and yield make TEBAL attractive for many applications including nanoelectronics, superconductivity, nanofluidics and molecular (DNA) translocation studies through nanopore-based transistors. References: 1) M.D. Fischbein and M. Drndic, "Sub-10 nm Device Fabrication in a Transmission Electron Microscope", Nano Letters, 7 (5), 1329, 2007. 2) M. D. Fischbein and M. Drndic, "Nanopacks by direct high-resolution imaging and electronic characterization of nanostructures", Applied Physics Letters, 88 (6), 063116, 2006.

3:06PM W35.00002 Atomic Precision in Nano-Electronics, DOUGLAS STRACHAN, DANVERS JOHNSTON, BETH GUITON, YE LU, SUJIT DATTA, PETER DAVIES, DAWN BONNELL, CHARLIE JOHNSON, University of Pennsylvania — One of the greatest challenges in developing molecular-scale devices is to fabricate and monitor their formation with atomic precision. Recently, we have developed an electromigration technique that employs feedback for controllably electromigrating a nano-scale electrode with atomic precision at room temperature [1]. We will discuss our recent progress advancing this technique towards atomically precise nano-electronics. This will include in-situ transmission electron microscopy which shows evidence for highly crystalline electrode formation and the parallel fabrication of nanoscale devices, and scaling-up to very large-scale integrated-circuits. Our results have implications on the development of a wide range of novel molecular-scale devices. Funding provided by: NSF-NSEC/NBIC DMR-0425780, NSF-NIRT Grant No. 0304531, and MRSEC award No. DMR05-20020. [1] D. R. Strachan, et al., Appl. Phys. Lett. 86, 043109 (2005).

3:18PM W35.00003 Quantifying the properties of nano-composites. MURRAY DAW, BO ZHANG, JIAN HE, TERRY TRITT, Clemson University — With the proliferation of nano-composites produced for possible thermoelectric application, we ask the question: To what extent is a given nano-composite like other composites? Or, in other words, when do we know that we have something new? To address this we apply the classical theory of composites to specific nano-composites grown and characterized at Clemson. The theory is very simple and assumes essentially very simple properties of the materials, the most important being Fourier's Law/Ohm's Law. Given this assumption, the theory of composites can be applied to the nano-composites based on what is known of the microstructure. This "classical" result then forms the basis by which the properties can be compared to determine if non-classical effects are being observed. One simple theory is the application of rigorous bounds, such as the Hashin-Strikman Bounds which are based only on very simple microstructural descriptors. Another simple theory is the application of FEM, which can be constructed directly from SEM images of the samples using the NIST code "OOF". The FEM produces specific predictions for the composite properties. We find that the Hashin-Strikman Bounds are very useful for analyzing the thermal conductivities of composites composed of metals and insulators, while the SEM technique can be applied successfully.

3:30PM W35.00004 ‘Focused Assembly’ of V$_2$O$_5$ Nanowires for Fabrication of Metallic Nanowire Sensors, TAE HYUN KIM, SUNG MYUNG, KWANG HEO, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University, HND TEAM — We present a method named ‘focused assembly’ for high-precision assembly of pristine V$_2$O$_5$ nanowires (NWs) on solid substrates. In this method, ‘microscale’ self-assembled monolayer patterns with ‘gradient’ surface molecular density ‘focused’ the assembly of V$_2$O$_5$ NWs onto the ‘nanoscale’ regions on a metallic thin film just like a lens focuses the light. The assembled NWs could be utilized as a shadow mask during the ion-milling process to generate metallic NW-based devices. As a proof of concepts, we successfully demonstrated the fabrication of metallic NW-based sensors to detect thiols molecules or hydrogen gas under ambient conditions. This focused assembly phenomenon gives us new insights about the directed assembly process of nanostructures. Furthermore, this approach provides us an easy, but efficient, means to mass-produce NW-based devices for various practical applications such as field effect transistors, chemical sensors and nanoscale interconnectors.

3:42PM W35.00005 Nanomechanical Spectroscopy: A novel route to label-free chemical sensing, PETER GREANEY, JEFFREY GROSSMAN, Center of Integrated Nanomechanical Systems, U. C. Berkeley — We propose a novel spectroscopic technique in which the vibrational modes of an analyte molecule are probed directly using a nanoscale mechanical resonator. It is anticipated that such “nanomechanical spectroscopy” can provide a method for label free chemical sensing. We elucidate the concept of the nanomechanical spectroscopy with the example of using an array of carbon nanotubes to detect a series of simple test molecules. In these examples, energy is transferred between the molecular vibrations of the analyte and specific phonon modes of the carbon nanotubes. Molecular dynamics simulations are used to explore the feasibility of this energy exchange for chemical sensing, and limits of both sensitivity and selectivity.

3:54PM W35.00006 ‘Lens’ Effect in Directed Assembly of Nanowires on Gradient Molecular Patterns, MOON GYU SUNG, SUNG MYUNG, JIWOO IM, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University, HND TEAM — We report a new phenomenon, named here as the ‘lens’ effect, in the directed-assembly process of nanowires (NWs) on self-assembled monolayer (SAM) patterns. In this process, the adsorption of NWs is focused in the nanoscale regions at the center of microscale SAM patterns with gradient surface molecular density just like an optical lens focuses light. As a proof of concepts, we successfully demonstrated the massive assembly of V$_2$O$_5$ NWs with single-walled carbon nanotubes (swCNTs) with a nanoscale resolution using only microscale molecular patterning methods. This work provides us with important insights about the directed-assembly process, and from a practical point of view, it allows us to generate nanoscale patterns of NWs over a large area for mass fabrication of NW-based devices.

4:06PM W35.00007 In$_2$O$_3$ Nanoparticles for Gas Sensors, ZENXCING ZHANG, DANIELA CARUNTU, CHARLES J. O’CONNOR, WEILIE ZHOU, Advanced Materials Research Institute, University of New Orleans, New Orleans, LA 70148 — In the last decades, sensors based on nanostructured materials have attracted much attention. Generally, nanosensors often demonstrate excellent sensitivities because of their high specific surface area and comparable size to the detected targets (chemicals or biomolecules). So far, lots of efforts have been put on the fabrication of nanowires based nanosensors. In this talk, we reported our recent work on employing wet-chemically synthesized indium oxide (In$_2$O$_3$) nanoparticles for gas sensing. The nanoparticles were self-assembled between the gold electrodes patterned on silicon substrates covered with thermal oxide film using e-beam nanolithography. Several gases, such as ammonia (NH$_3$), hydrogen sulfide (H$_2$S), etc., were used for the testing. The results exhibit that the sensitivity can be reached down to PPM order. In addition, the sensitivity in terms of nanoparticle size, temperature, etc., were also investigated.
4:18PM W35.00008 Environment of TiO\textsubscript{2} nanoparticles as an important factor to achieve highly efficient on dye sensitized solar cells\textsuperscript{1}, TEREZA PARONYAN, M.C. LIN, DEPT. OF APPLIED CHEMISTRY, NATIONAL CHIAO TUNG UNIV. TEAM, INST. FOR PHYSICAL RESEARCH, NAAS, ASHTAFAR, ARMENIA COLLABORATION, DEPT. OF CHEMISTRY, EMORY UNIV. COLLABORATION — Amorphous TiO\textsubscript{2} nanoparticles were synthesized through sol gel technique. Environment of nanoparticles was neutralized by ammonia, and pH 5.8 of TiO\textsubscript{2} gel was achieved in result, which is close to the point of zero charge (PZC) of anatase TiO\textsubscript{2}. Highly interconnected, mesoporous, transparent films were fabricated from the TiO\textsubscript{2} colloid with pH 5.8. AFM, SEM XRD analyses were carried out for the investigation the size of nanoparticles, the surface morphology and the crystal structure of films. Volt-ampic characteristics showed an improvement in the cell efficiency along with the increasing of pH TiO\textsubscript{2} colloid. The cells parameters (Voc, FF, Jsc, η) were studied depending on the pH of TiO\textsubscript{2} colloid. Increasing pH of the colloid from 2.1 to 5.8 enhanced the overall conversion efficiency of the dye-sensitized solar cells by approximately 30\%, and 9.2 \% of efficiency was achieved with N719 dye under illumination by simulated AM1.5 solar light (100 mW/cm\textsuperscript{-2}).

\textsuperscript{1}This work was financially supported by 952001INER027 and 962001INER0029 Solar Energy Projects of Taiwan. The authors thank to Prof. A.M. Kichhtian for discussions.

4:30PM W35.00009 Electron Thermal Microscopy of Multiwalled Carbon Nanotubes , KAMAL BALOCH, TODD BRINTLINGER, JOHN CUMINGS, University of Maryland — A thorough electrical and thermal characterization of carbon nanotubes (CNTs) is essential for their application as electrical and thermal devices. We demonstrate high-resolution thermal imaging of multiwalled CNT using electron thermal microscopy. This is achieved by observing the solid to liquid phase transition of low melting point indium islands in a transmission electron microscope. High resolution thermal maps thus obtained provide a qualitative analysis of transfer of heat along a CNT suggesting a trend of CNT acting as a heat spreader. Also, important parameters like thermal conductivity of the CNT can be extracted by finite element modeling. The temperatures involved are \sim 200C and the samples can be operated over several voltage cycles. Experimental technique, high resolution maps, real time videos, and simulation results will be presented.

4:42PM W35.00010 The Nuclear Environment for Electron Spins in a Double Quantum Dot\textsuperscript{1}, DAVID REILLY, Harvard University, JACOB TAYLOR, MIT, JASON PETTA, Princeton, CHARLES MARCUS, Harvard, MICAH HANSON, ART GOSSARD, UCSD, HARVARD COLLABORATION, UCSD COLLABORATION — We report measurements examining the nuclear spin environment for electrons in a GaAs double quantum dot. The hyperfine field, which drives transitions of a two-electron spin state, is detected via spin-to-charge transfer and rf-QPC readout. Fluctuations of the hyperfine field are measured to be broadband, with spectral content ranging from millisecond to the decoherence time of \sim 10 seconds. In addition, we demonstrate dynamic nuclear polarization (DNP) using a cyclic gate-pulse sequence. Relaxation of the DNP is studied using time-resolved measurements and found to be sensitive to the spin-state of electrons. The presence of a small DNP is found to suppress hyperfine fluctuations by a factor of \sim 100, leading to a time-ensemble dephasing time, T\textsubscript{2} \sim 1 microsecond for electron spins.

\textsuperscript{1}This work was supported by DARPA, DTO, NSF-NIRT (EIA-0210736) and Harvard Center for Nanoscale Systems. Research at UCSB supported in part by QuEST, an NSF Center.

4:54PM W35.00011 Nanoscale probing of material properties across antiparallel domain wall in ferroelectrics , VASUDEVA RAO ARAVIND, LILI TIAN, NOZOMI ODAKAWA, SAMRAT CHOUDHURY, PAVEL CAPEK, VOLKMAR DIEROLF, ANNA N. MOROZOVSKA, EUGENE A. ELISEEV, LONG-QING CHEN, YASUO CHO, SERGEI KALININ, VENKATRAMAN GOPALAN, Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA 16802, USA — Although the intrinsic width of an ideal antiparallel ferroelectric domain wall is expected to be step-like on a unit cell level (\sim 0.5nm), we have recently shown that actual widths of these walls can extend to \sim 200nm in lithium niobate and lithium tantalate (L.Tian et al., Physical Review Letters (in review)). In this work we study the variation of material properties coercive field and switchable ferroelectric polarization as a function of the distance from the domain wall in lithium niobate. Until recently, the study of these material properties on the nanoscale were limited by the lack of theoretical modeling of the instrument resolution limits. Using experimental results and theoretical modeling we demonstrate the relation between intrinsic width of the domain wall and its effect on material properties.

5:06PM W35.00012 Electrostatic and Nanotechnology Multidisciplinary Approach - for Space Radiation Shielding , RAM TRIPATHI, JOHN WILSON, NASA Langley Research Center, Hampton, VA 23681, ROBERT YOUNQUIST, NASA, The John F. Kennedy Space Center, FL 32899 — For the success of NASA's new vision for space exploration to Moon, Mars and beyond, exposures from the hazards of severe space radiation in deep space long duration missions is a "must solve" problem. The exploration beyond low Earth orbit to enable routine access of space will require protection from the hazards of the accumulated exposures of space radiation. There is a need to look to new horizons for newer technologies. The present multidisciplinary investigation explores the feasibility of using the active electrostatic shielding in concert with the state-of-the-art materials shielding and protection technologies. The full space radiation environment has been used, for the first time, to explore the feasibility of multidisciplinary shielding. The goal is to repel enough positive charge ions so that they miss the spacecraft without attracting thermal electrons and further attenuate the exposure using nano-materials. Conclusions are drawn for the future directions of space radiation protection.

5:18PM W35.00013 Probing Local Structures in ZrO\textsubscript{2} Nanocrystals Using EXAFS\textsuperscript{1}, Y.L. SOO, P.J. CHEN, S.H. HUANG, T.J. SHIU, T.Y. TSAI, Y.H. CHOW, Y.C. LIN, S.C. WENG, S.L. CHANG, National Tsing Hua University, J.F. LEE, NSRRC, Taiwan, C.L. CHEUNG, R.F. SABIRIANOV, F.N. NAMAVAR, F.W. MEI, University of Nebraska — Extended x-ray absorption fine structure (EXAFS) has been employed to investigate the local structures surrounding Zr in cubic zirconia thin films prepared by an ion beam assisted deposition technique. These materials have demonstrated promising mechanical properties such as improved hardness and lubricant wettability compared to yttria-stabilized zirconia. To verify the cubic structure of zirconia in films prepared under different growth conditions and to fully understand the mechanism leading to their unique physical properties, the structural information is a required prerequisite. Since zirconia is in the form of nanosized crystallites, conventional x-ray diffraction method is not useful for this purpose. Our x-ray results reveal cubic-like structure with O vacancies around Zr in several nanocrystal samples. Powders of cubic zirconia prepared using chemical methods were also measured for comparison.

\textsuperscript{1}This research is supported by NSC under project number 95-2112-M-007-014.

Thursday, March 13, 2008 2:30PM - 5:42PM — Session W36 DMP: Focus Session: Materials for Photovoltaics and Photocatalysis III

2:30PM W36.00001 TBD, DARIN LAIRD, Plextronics — This abstract not available.
3:06PM W36.00002 Hole Mobility Studies on Thiophene-Based Conjugated Polymers Developed for Use in Organic Electronic Devices , N.C. HESTON, Univ of Florida, Dept of Phys, J. MEI, Univ of Florida, Dept of Chem, D.B. TANNER, Univ of Florida, Dept of Phys, J.R. REYNOLDS, Univ of Florida, Dept of Chem — In optimizing organic electronic devices, such as solar cells and field effect transistors, the mobility plays a crucial role affecting many aspects of performance, including: charge separation efficiencies, carrier densities, and drain currents. By fabricating hole-dominated devices and fitting the measured current-voltage characteristics to the field-dependent space-charge-limited mobility model we were able to measure hole mobilities in a set of conjugated polymers including p-Pt-BTD-Th, p-Pt-BTD-EDOT, and both regio-regular and regio-random P3HT. These materials have been shown to exhibit promise as active layers in organic solar cells, light-emitting diodes, and field effect transistors. We present the results of these measurements and the effects induced by thermal annealing.

3:18PM W36.00003 Molecular and electronic structure at C_{60}/pentacene interfaces , S.W. ROBEY, D.B. DOUGHERTY, NIST-Gaithersburg, W. JIN, W.G. CULLEN, G.J. DUTTON, J.E. REUTT-ROBEY, University of Maryland — Successful utilization of organic donor-acceptor systems for photovoltaic applications requires understanding factors controlling molecular and electronic structure at interfaces. We have used STM, STS, and photoemission to study the donor-acceptor system C_{60}/pentacene. At low coverage, C_{60} is deposited on a well-ordered pentacene bilayer structure on Ag (111) adsorbs in between two adjacent pentacene rows. Isolated C_{60} molecules are easily observed at room temperature indicating that the mobility of C_{60} on pentacene is significantly smaller than on metal surfaces. Some images of C_{60} reveal structure that may indicate a preferred C_{60} orientation. Electrostatic contributions to intermolecular interactions are discussed to help explain C_{60} adsorption between pentacene molecules. With increasing coverage, C_{60} forms linear chains, still locked to underlying pentacene rows. A further increase in coverage results in domains of disordered C_{60} that we propose result from competing C_{60}− C_{60} and C_{60}/pentacene interactions. Information on nanoscale transport gaps and band alignment was obtained using constant-current distance-voltage spectroscopy. A gap of 4.5 eV is found over the linear C_{60} chains compared with a gap of 3.6 eV for the surrounding pentacene bilayer.

3:30PM W36.00004 Porous nanocrystalline TiO_2 thin films for dye-sensitized solar cells , XI-AOJUAN FAN, Marshall University, CLAUDIA SWANSON, DAVID ROGOW, University of California, AKHILESH TRIPATHI, Rigaku Corporation, SCOTT OLIVER, University of California — We report a rapid and low cost method to fabricate porous TiO_2 thin films used as anode electrodes for solid state dye-sensitized solar cells. Polymethylmethacrylate (PMMA) gel was used as template to define a network co-structure with alkali titanium oxide, then spin cast on substrates. After removing polymer, smooth and crack-free large area TiO_2 thin films with fine pores were generated. Thin film structures were detected by powder & grazing incident X-ray diffraction. Thickness can be controlled over a range of tens of nanometers to several microns by precursor viscosity, spin coating speed and coating times. The SEM image shows the highest quality porous TiO_2 film derived from a certain concentration of precursor. The above TiO_2 thin films were then used to fabricate solid state dye sensitized solar cells. Porphyrine dye and poly(ethylene glycol) electrolyte with I^-/I_3^- redox couple were used in the cells. Current−voltage curves were recorded. The open circuit voltage boosts to more than 1.0 V. The reasons for the high open circuit voltage probably will be discussed. Overall photo-electricity conversion efficiency reaches 2.05% under an illumination of one solar unit (AM1.5, 100 mW/cm^2).

3:42PM W36.00005 TiO2 nanowire sensitized by natural dyes for solar cell applications , SHENG MENG, JUN REN, EFTHIMIOS KAXIRAS, Harvard University — We investigate the electronic coupling between a semiconductor TiO_2 nanowire and a natural dye sensitizer based on time-dependent first-principles calculations. The model dye molecule, cyanidin is found to dissociate into the quinonoidal form upon adsorption, rendering its highest occupied molecular orbitals (HOMO) located in the middle of TiO_2 bandgap and its lowest-unoccupied molecular orbital (LUMO) at the bottom of TiO_2 conduction band. The visible light absorption is greatly enhanced with two prominent peaks at 460 nm and 650 nm. The excited electrons are injected into the TiO_2 conduction band within a ultrafast timescale of <50 fs, with negligible non-radiative energy dissipation and recombination.

3:54PM W36.00006 Electronic structure of N3 DYE molecules on the TiO_2(110) surface and on anatase nanoparticle films , ERIC, BERSCH, Rutgers University, SYLVIE RANGAN, University of Texas at Dallas, JEAN-PATRICK THEISEN, ROBERT A. BARTYNSKI, JUDITH D. SORGE, DUNBAR P. BIRNIE, Rutgers University — We have used direct and inverse photoemission to measure the occupied and unoccupied electronic states, and their alignment with the band edges of the substrate, of N3 dye adsorbed on the rutile TiO_2(110) surface and on anatase TiO_2 nanoparticle thin films. In dye-sensitized solar cell applications, the HOMO-LUMO gap determines the useful portion of the solar spectrum, and charge transfer of photoexcited electrons to the substrate depends on the alignment of the LUMO to the TiO_2 conduction band edge. Samples were prepared and passivated with a pivalate layer in UHV, then sensitized in air in a solution of N3 dye in acetonitrile. STM measurements show that the pivalic acid forms an ordered overlayer on the TiO_2(110) surface and that the N3 dye molecules can be imaged after sensitization. Our spectroscopic measurements show that contamination (presumably from water in the ambient) is significantly reduced and that the N3 HOMO occurs at 1.1 eV above the TiO_2 valence band edge. The LUMO of the TiO_2 is found at 0.3 eV above the conduction band edge. Comparison with experimental and theoretical values from the literature will be discussed.

4:06PM W36.00007 Electronic structure of N3 DYE molecules on the ZnO single crystal and epitaxial film surfaces , JEAN-PATRICK THEISEN, ERIC BERSCH, SYLVIE RANGAN, YICHENG LU, ROBERT BARTYNSKI — Most dye-sensitized solar cells use TiO_2 nanoparticle films as the electrode, but ZnO offers an interesting alternative. We have used direct and inverse photoemission to measure the occupied and unoccupied electronic states, and their alignment with the band edges of the substrate, of N3 dye adsorbed on ZnO(0001), ZnO(11-2), epitaxial ZnO a-plane film surfaces, and ZnO nanopillars. As the unoccupied states of ZnO are of sp-character and of relatively low cross section, the LUMO of the dye is easily observed. Samples were prepared and passivated with a pivalate layer in UHV, then sensitized in air in a solution of N3 dye in acetonitrile. As opposed to the case of the TiO_2(110) surface, STM measurements indicate that the pivalic acid does. From UPS, the N3 HOMO is found at ~0.8 eV above the ZnO valence band edge, and the LUMO is found ~1.5 eV above the conduction band edge for the epifilm. Differences in dye adsorption and orbital alignment for these different ZnO surfaces will be discussed.

4:18PM W36.00008 Towards visible light activity of wide band gap photocatalysts: Surface functionalization of ZnO with ZnS , JAYEETA LAHIRI, MATTHIAS BATZILL, Department of Physics, University of South Florida, Tampa, FL 33620 — We show that at the ZnO/ZnS interface the band alignment is favorable for reducing the photo excitation threshold energy; signifying that the combination of two wide band gap photocatalysts can yield a material with visible light activity. Modification of ZnO with a sub monolayer ZnS is investigated by scanning tunneling microscopy (STM) and photoemission spectroscopy. STM studies indicate that the ZnS grows by nucleation and spreading of 2D clusters of monolayer height (~ 2.5 Å). Photoemission spectroscopy is used to measure the band alignment between ZnO and ZnS, as well as measure the changes in the surface charge region and work function. An increase in work function by 1.1 eV is observed and a staggered band alignment is found with ZnS states effectively narrowing the band gap for photo excitation from 3.4 to 2.7 eV. We propose that the combination of these structural and electronic properties of the modified ZnO surface result in an improved, visible light active photocatalyst.
4:30PM W36.00009 Energy bands and point defects in CuInSe₂ and CuGaSe₂ calculated by Quasiparticle Self-Consistent GW. 
MARK VAN SCHILFGAARDE, TAKAOK KOTANI, Arizona State University — CuIn_xGa_1−xSe_2, or CIGS, is emerging as a leading candidate for second-generation solar cell applications. Here we present the bulk energy band properties and dielectric response of CuInSe₂ and CuGaSe₂, computed within the Self-Consistent GW (QSGW) approximation. QSGW has been proven to be a reliable, true ab initio predictor of QP levels in a wide variety of materials systems; it is expected to be similarly reliable for chalcoprite semiconductors. The fundamental gap agrees well with experiment. Also, the electron and hole effective masses are evaluated. Various kinds of point defects were considered using certain approximations to QSGW. Of particular interest are low-energy cation defects (antisites and vacancies). Rather unusual properties of these levels are found, owing to the unique role that shallow Cu d states play in CIGS.

4:42PM W36.00010 Synthesis of type II core/shell nanowires for photovoltaic application, WEILIE ZHOU, KAI WANG, JIAJUN CHEN, Advanced Materials Research Institute, University of New Orleans, YONG ZHANG, JOHN PERN, YANFA YAN, ANGELO MASCARENHAS, National Energy Renewable Laboratory, NATIONAL ENERGY RENEWABLE LABORATORY COLLABORATION — The core/shell semiconducting nanowires based on II-VI semiconductors, involving with type II band energy alignments, are predicted to be a new kind of nanostructured materials for efficient charge separation for stable and efficient photovoltaic devices. In this talk, we report a successful synthesis of II-VI semiconducting core/shell nanowires by a relatively simple and low-cost approach. The structures and optical properties were characterized by applying a set of comprehensive techniques. A sharp interface and the epitelial relationship between the core and shell were observed. Two excitonic absorption peaks were clearly found at respective excitonic bandgaps, indicating a good crystallinity of both the core and shell. Compared to the single component nanowires, the PL spectrum of the core/shell nanowires shows a reduction in intensity and a slight blue shift at the band edge emission of the core nanowires, which may partially arise from spatially charge separation between the core and shell. The direct growth of core/shell nanowires represents a major step toward fabricating a low-cost, high efficiency and stable solar cell.

5:45PM W36.00011 Nanocoax Solar Cells, M.I. NAUGHTON, K. KEMPA, Z.F. REN, J. RYBCZYNSKI, T. PAUDEL, Y. GAO, Y. XU, Boston College — A novel architecture for high efficiency solar energy conversion, employing separated photo– and –voltaic pathways and vertically-aligned, nanoscale, metallic coaxial wires (nanocoax) which are indeed simultaneously thick (tall) and thin (narrow). Photons captured by nanoscale antennas are channeled axially as TEM-mode radiation in the nanocoax annulus, which is filled with a PV medium. This annulus is unprecedentedly thin radially (~100 nm), such that exciton lifetimes and subsequent electron and hole diffusion lengths of virtually any PV material are sufficiently long to enable highly efficient solar energy conversion. We discuss results with radial p – i – n junctions using α-Si PV and carbon nanofiber coax center conductors, where nanocoax solar cell efficiencies exceed those of comparable planar junctions. Moreover, this nanoscale architecture can be considered a feasible portal to 3rd generation solar power.

5:06PM W36.00012 Low temperature pulsed electrically detected magnetic resonance on a-Si:H p-i-n solar cells, THOMAS HERRING, HEATHER SEIPEL, DANE MCCAMEY, CHRISTOPH BOEHME, University of Utah, CRAIG TAYLOR, Colorado School of Mines, JIAN HU, FENG ZHU, ARUN MADAN, MV Systems, Golden, CO — Hydrogenated amorphous silicon (α-Si:H) has become one of the most important semiconductor materials, with applications including solar cells and thin film transistors. In spite of this, and more than 30 years of intensive studies of this material, the microscopic nature of various recombination mechanisms in this material are still not well understood. Recently, pulsed electrically and optically detected magnetic resonance (p-EDMR, p-ODMR, respectively) spectroscopy has provided a method for directly and quantitatively observing some of these microscopic processes. Here, we present p-EDMR measurements on a-Si:H p-i-n solar cells at temperatures T ≤ 40K, with a comparatively low light intensity. After a short, coherent microwave excitation, we record transients for a range of externally applied magnetic fields. The results show the presence of a number of resonances, which we discuss with regard to previous continuous wave (cw-) ESR and cw-EDMR studies, as well as cw- and p-ODMR measurements.

5:18PM W36.00013 Carrier Multiplication in Semiconductor Nanocrystals: Theoretical Screening of Candidate Materials, JUN-WEI LUO, ALBERTO FRANCESCHETTI, ALEX ZUNGER, National Renewable Energy Lab — The process of Direct Carrier Multiplication (DCM) involves the creation of two electron-hole pairs as a result of exciting a nanostructure by one photon with energy two times larger than the band gap 

5:30PM W36.00014 Exploring the Use of Self-Assembled InGaAs/GaAsP Quantum Dots as Intermediate Band Solar Cells (IBSC) , VOICIU POPECU, GABRIEL BETSTER, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO — It has been recently proposed that the efficiency of photovoltaic solar cells based on wide-gap III-V absorbing materials can be enhanced if quantum dots are embedded in such structures, leading to confined electron and hole states that can be excited to the band edges of the wider-gap matrix material, thereby capturing the lower energy (IR) solar photons. Such proposals, however, were not scrutinized so far by modern quantum-dot calculations. We apply our pseudopotential Linear-Combination-of Bloch-Bands (LCBB) approach to this problem. Lens-shaped dots of InGaAs were vertically stacked with varying dot-dot separation. The effects of spin-orbit, multi-band, and multi-valley coupling are included by a direct diagonalization of the atomistic problem. Lens-shaped dots of InGaAs were vertically stacked with varying dot-dot separation. The ratio 

The effects of spin-orbit, multi-band, and multi-valley coupling are included by a direct diagonalization of the atomistic problem. A matrix of GaAsP was chosen so as to strain-balance the system epitaxially on a GaAs(x) substrate. We will discuss the energies of the band edges of the matrix material, and those of the confined dot levels relative to the expected values for ideal IBSC operation, as well as their variation with respect to either the vertical dot-dot separation, or the band gap of the matrix material.

Funded by DOE-SC-BES-DMS
Max Planck Institute for Solid State Research, Stuttgart, Germany

Thursday, March 13, 2008 2:30PM - 5:30PM — Session W37 DCMP: Focus Session: Multiferrocity in BiFeO₃-based films — Morial Convention Center
2:30PM W37.00001 First-principle calculations of electronic structure of bismuth ferrate and manganate with the mullite structure. JEN-CHANG CHEN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617, Taiwan — We applied ab initio total-energy calculation to study the electronic structure of Bi$_2$Fe$_2$O$_5$ and Bi$_2$Mn$_2$O$_6$ single crystals. Both crystals are orthorhombic with the centro-symmetric structure and belong to the mullite-type material. Most of bismuth-based oxides exhibit good ferroelectricity, pyroelectricity and piezoelectricity. However, little researches of electronic structure and properties have been done on the bismuth ferrate and bismuth manganate. In this study, we band structure, density of state, partial density of state and magnetic moment of both bismuth ferrate and bismuth manganate at zero Kelvin were calculated. The effect of Fe and Mn atom within the structure were discussed. The phase stability of these two crystals was also examined.

2:42PM W37.00002 The structural, magnetic, and electric properties of Sr and Ca-doped BiFeO$_3$ films. CHAN-HO YANG, M. HUIJBEREN, Y.-H. CHU, L.W. MARTIN, M. HOLCOMB, R. RAMESH, Department of Material Science Engineering and Department of Physics, University of California, Berkeley, M. CHI, N. BROWNING, Department of Materials Science and Engineering, University of California, Davis — Many perovskite oxides, as holes are doped, exhibit unusual physical phenomena such as superconductivity, colossal magnetoresistance, metal-insulator transition, and charge ordering. We are exploring the consequences of hole doping into a well known multiferroic, the antiferromagnetic ferroelectric, BiFeO$_3$. In this presentation, the systematic investigation on structural, electronic, and magnetic properties will be presented for nominally hole-doped BiFeO$_3$ obtained by partially substituting Ca for Sr and Sr for Ca. The ordering of ferroelectricity and magnetic ordering at room temperature, has polarization along [111] direction and is a G-type antiferromagnet. The divalent ion doping weakens the ferroelectric properties but improves magnetization owing to cluster-glass-like magnetism. We will discuss the magnetic properties based on superexchange mechanism. The structural characterization by X-ray diffraction, scanning microscopy and TEM will be presented. The SQUID and the dielectric constant measurements as a function of magnetic field and temperature will be also reported.

2:54PM W37.00003 Phase diagram for Bi$_{1-x}$Ca$_x$MnO$_3$ (x < 0.4). YUHAI QIN, TREVOR TYSON, New Jersey Institute of Technology, SANG-WOOK CHEONG, Rutgers University, XIAO-NONG XU, Nanjing University — The multiferroic BiMnO$_3$ system, in which ferroelectric and ferromagnetic orders can coexist, has attracted much research work in the past years for its potential technological applications. For the more general system Bi$_1-x$Ca$_x$MnO$_3$, the phase diagram for the Ca rich region (x < 0.4) has been established[1]. In order to understand the multiferroic behavior near the x=0 system, the hole-doped region (0<x<0.4) was investigated. We have completed the magnetic, transport, and structural phase diagram of Bi$_1-x$Ca$_x$MnO$_3$, by performing detailed structural (XRD and XAFS) and electrical measurements on Bi$_1-x$Ca$_x$MnO$_3$ (0<x<0.4), showing the transition form the highly distorted monoclinic phase to the orthorhombic phase. This work is supported by NSF DMR-0512196 and DOE Grant DE-FG02-07ER46402. [1] H. Woo, et al, Phys. Rev. B: Condensed Matter and Materials Physics 63, 134412/1 (2001).

3:06PM W37.00004 Combinatorial discovery of morphotropic phase boundary in a lead-free high $T_c$ piezoelectric perovskite Bi$_{1-x}$(RE)$_x$FeO$_3$. F. FUJINO, D. KAN, A. VARATHARAJAN, C.J. CHENG, V. NAGARAJAN, M. MURAKAMI, S.-H. LIM, D. HUNTER, C.J. FENNIE, L. SALAMANCA-RIBA, M. WUTTIG, I. TAKEUCHI — We have recently discovered a morphotropic phase boundary (MPB) in Bi$_{1-x}$Sm$_x$FeO$_3$ which has a simple perovskite structure. We have systematically investigated compositionally varied Sm doped BiFeO$_3$ thin films using the combinatorial approach and found that ferroelectric properties and piezoelectric properties show pronounced enhancement at the MPB. The samples were fabricated by combinatorial pulsed laser deposition on SrTiO$_3$ (001) substrates with a SrRuO$_3$ buffer layer. The boundary is a rhombohedral to pseudo-orthorhombic structural transition which exhibits a ferroelectric to antiferroelectric transition at approximately $T_{mp}$=120 K, intrinsic $d_33$ comparable to those of PbZr$_{0.52}$Ti$_{0.48}$O$_3$ thin films. Transmission electron microscopy (TEM) reveals presence of nanodomains at the MPB. TEM also reveals onset and formation of antiferroelectric domains as the composition is swept near the MPB, where electron diffraction patterns show systematic structural tilt transitions of the system as a function of Sm doping. Finally, we report on structural transitions and ferroelectric properties in other Bi$_{1-x}$(RE)$_x$FeO$_3$ systems systematically studied by the composition spread technique. This work is supported by NSF MRSEC, AR0, and the W. M. Keck Foundation. Research at UNSW is supported by DEST Australia, Australian Research Council Grant DP 0666231 and ARNAM Travel Grant.

3:18PM W37.00005 The effect of structural and chemical perturbations in multiferroic BiFeO$_3$ epitaxial films. DAE HO KIM, H.N. LEE, M. VARELA, H.M. CHRISTEN, Mat. Sci. and Tech. Div., Oak Ridge Nat. Lab., Oak Ridge, TN, M.D. BIEGALSKI, Center for Nanophase Mat. Sci., Oak Ridge Nat. Lab., Oak Ridge, TN, C.J. CALLENDE, D.P. NORTON, Dept. of Mat. Sci. & Engr., Univ. of Florida, Gainesville, FL — The compatibility between the lone-pair driven ferroelectric distortion and antiferromagnetic order in BiFeO$_3$ attracts a lot of attention. A detailed understanding of ferroelectric properties in BiFeO$_3$ is gained by investigating the effect of structural/chemical perturbations in strained epitaxial films with chemical modifications. Our work shows that the ferroelectric polarization along [111] exhibits weak dependency on epitaxial strain on a (001) substrate. A detailed examination of role induced by magnetic ions, we have grown BiFe$_{1-x}$Cr$_x$O$_3$ epitaxial films and observed a ferroelectric to antiferroelectric transition with increasing the Cr content. Furthermore, epitaxial films of Bi$_{1-x}$Ba$_x$FeO$_3$ were grown to investigate the effect of structural variation in connection with change in the valence of Fe ion. The results reveal a high stability of the ferroelectric distortion in epitaxial BiFeO$_3$ films.

3:30PM W37.00006 Structural, electrical and magnetic properties of Bi(Fe$_{1-x}$Ti$_{1-x}$)O$_3$ thin films. N.M. MURARI, R. MELGAREJO, R. THOMAS, R.S. KATIYAR, Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, P.O. Box 23343, PR 00931 — Multiferroic materials have recently seen a surge of research activities due to its applications in the memory, spintronics, sensors devices and micro mechanical systems (MEMS). BiFeO$_3$ is a naturally occurring multiferroics. However, the large leakage current is a concern for practical applications and substitution at Bi and Fe is commonly employed to circumvent this problem. Here, Fe substitution by Ti is considered for this purpose. Thin films on Pt/Ti/SiO$_2$/Si were grown by chemical solution deposition (CSD) and characterized for structure and symmetry by XRD and Raman scattering, surface morphology by AFM, dielectric properties by impedance analyzer, and the leakage current by I-V measurements. Magnetic (M-H) and electric (P-V) hysteresis loops were also studied. Variation of dielectric constant (e') and loss tangent (tanδ) with temperature, frequency and temperature were systematically studied. Further, the effect of Ti substitution on the electrical properties will be presented.

3:42PM W37.00007 Piezoelectricity and structure of epitaxial ferroic thin films at high electric fields. ALEXEI GRIGORIEV, RIBECCA SICHIEL, University of Wisconsin-Madison, HO NYUUNG LEE, Oak Ridge National Lab, CHANG-BEOM EOM, University of Wisconsin-Madison, ZHONGHOU CAI, ERIC C. LANDAHL, BERNHARD ADAMS, ERIC M. DUFRESNE, Argonne National Lab, PAUL G. EVANS, University of Wisconsin-Madison — With mastering the techniques to grow nearly perfect epitaxial thin oxide films, there are emerging opportunities to control the structure and properties of oxide materials using extremely high electric fields. To unveil the piezoelectric and structural properties of Pb(Zr,Ti)O$_3$ and BiFeO$_3$ epitaxial thin films at electric fields which are a few times stronger than the low-frequency dielectric breakdown field, we employed time-resolved structural measurements synchronized with electric field pulses of a nanosecond duration. At these extreme fields we measured record-high piezoelectric strains and explored nonlinearities in piezoelectric responses predicted to occur due to the changes in interatomic interactions.
3:54PM W37.00008 Giant Polarization Rotation in BiFeO$_3$/SrTiO$_3$ Thin Films,

M.C. LANGNER, Y.H. CHU, L.M. MARTIN, M. GAJEK, R. RAMESHI, J. ORENSTEIN, UC Berkeley, LBNL — We use optical second harmonic generation to probe dynamics of the ferroelectric polarization in (111) oriented BiFeO$_3$ thin films grown on SrTiO$_3$ substrates. The second harmonic response indicates 3m point group symmetry and is consistent with a spontaneous polarization normal to the surface of the film. We measure large changes in amplitude and lowering of symmetry, consistent with polarization rotation, when modest electric fields are applied in the plane of the film. At room temperature the rotation is an order of magnitude larger than expected from reported values of the dielectric constant and increases further (as 1/T) as temperature is lowered. We propose a substrate interaction model to explain these results.

3This work supported by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, DOE

4:06PM W37.00009 ABSTRACT WITHDRAWN —

4:18PM W37.00010 Exchange biasing with multiferroic: electric field effects on magnetic and magnetotransport properties.

J. FONTCUBERTA, Institut de Ciencia de Materials de Barcelona-CSIC, Campus UAB, Bellaterra 08193, Catalonia, Spain — Room-temperature multiferroic materials are scarce and display a weak magnetoelectric coupling and thus huge difficulties exist for controlling the magnetic state by using an electric field or viceversa. A possible alternative to circumvent this limitation is to exploit the clamping of ferroelectric and antiferromagnetic domains in biferroic materials and use a suitable exchange-bias existing with ferromagnetic materials to tune the magnetic response of the ferromagnet. In this presentation we shall overview recent experiments on exchange-biasing using hexagonal YMN$_2$ biferroics and Permalloy as a soft-ferromagnet. Exchange-bias on ferromagnetic materials is most commonly evidenced by their magnetic response, although magnetotransport measurements are also very adequate to monitor the exchange bias. We will present and discuss first how exchange-bias is manifested and monitored. Next, we will describe the effects of an electric field, biasing the ferroelectric (and antiferromagnetic) epitaxial layer, on the exchange bias. We will show that under appropriate conditions, magnetization can be switched by application of a suitable electric field. We will discuss the significance of the results with particular attention to role of current leakages across the ferroelectric.

In collaboration with X. Martí, Institut de Ciencia de Materials de Barcelona-CSIC, Spain; V. Laukhin, Institut de Ciencia de Materials de Barcelona-CSIC and Institut Català de Recerca i Estudis Avançats (ICREA), Barcelona, Catalonia, Spain; V. Skumryev, Institut Català de Recerca i Estudis Avançats (ICREA) and Departament de Física, Universitat Autònoma de Barcelona, Spain; D. Hrabovsky and F. Sánchez, Institut de Ciencia de Materials de Barcelona-CSIC, Spain; M. Varela, Departament de Física Aplicada i Óptica, Universitat de Barcelona, Spain; U. Lüders and J.F. Bobo, LNMH ONERA-CNRS, France.

4:54PM W37.00011 Investigation of the electrical switching of magnetization through exchange interactions with a magnetoelectric multiferroic.

A. LEE, ALEX DE LOZANNE, University of Texas at Austin, YING-HAO CHU, LANE W. MARTIN, MIKÉL BARRY, QIAN ZHAN, KILHO LEE, Z. Q. QIU, R. RAMESHI, University of California, Berkeley — The coupling between antiferromagnetic (AF) and ferromagnetic (FM) ordering at an interface between the two types of materials has been well established and provides the basis for modern day hard drives. BiFeO$_3$ is a magnetoelectric multiferroic material which shows coupling between ferroelectric (FE) and AF phases. The Curie and Neél temperatures are $\sim$820 and 370 °C, respectively, permitting room temperature operation. Manipulation of the FE ordering via external electric fields affects the AF ordering which in turn permits control over the magnetization of an adjacent FM material. We present the results of our investigation into the control of magnetic domains using electric fields. The object of investigation is a multilayer film of Co$_{30}$Fe$_{30}$Fe$_{30}$/BiFeO$_3$/SrRuO$_3$/SrTiO$_3$(001) patterned into islands. A magnetic force microscope is used both to image the magnetic domains and to apply the potential across the film.

5:06PM W37.00012 Anisotropic photo-control of spontaneous polarization in BiFeO$_3$ thin films: Indications of photo-assisted magnetoelectric effect.

D.S. RANA, I. KAWAYAMA, H. MURAKAMI, M. TONOUCHI, Institute of Laser Engineering, Osaka University, JAPAN TEAM — The terahertz (THz) emission from multiferroic BiFeO$_3$(BFO) due to ultra-fast depolarization of electric order helps in evaluating its ferroelectric behavior [1]. In this work, we investigate THz-emission in BFO films on (LaAlO$_3$)$_{0.7}$(Sr$_3$Al$_2$O$_6$)$_{0.3}$ (LSAT) substrates along (100), (110) and (111) directions. THz emission amplitude ($E_{THz}$) and its electric field dependence are similar in BFO (100) and BFO (110): $E_{THz}$ as function of electric field translates to ferroelectric-like hysteresis loop, and sign and amplitude of THz-emission are commensurate with the applied electric field. On the contrary, in BFO (111) the hysteretic loop is absent, $E_{THz}$ varies linearly with electric field and the polarity of THz-emission is opposite to that of the electric field. These results suggest that THz-emission is mainly a result of ultrafast depolarization but with a superimposed character of ultrafast reorientation or demagnetization of antiferromagnetic (AFM) order. Though AFM order in BFO makes the determination of magnetoelectric (ME) coupling rather difficult, the photo-assisted electric field control of AFM order shown in the present work is suggestive of photo-assisted ME effect. 1. K. Takahashi et al., Phys. Rev. Lett. 96, 117402 (2006).

5:18PM W37.00013 Measurements of Bandgap of Epitaxial BiFeO$_3$ Films by UV-VIS Absorption and Cathodoluminescence Spectroscopies.

A.J. HAUSER, Department of Physics, The Ohio State University, Z. JHANG, Department of Electrical Engineering, The Ohio State University, L. MIER, R. RICCIARDO, P.M. WOODWARD, T.L. GUSTAFSON, Department of Chemistry, The Ohio State University, L.J. BRILLSON, Department of Electrical Engineering, The Ohio State University, F.Y. YANG, Department of Physics, The Ohio State University — We report measurements of the bandgap of pure-phase epitaxial BiFeO$_3$ thin films on (001)-oriented SrTiO$_3$ substrates, via UV-VIS absorption and cathodoluminescence (CL) spectroscopies. 70 nm thick BiFeO$_3$ films were grown using ultrahigh vacuum RF magnetron sputtering at substrate temperatures between 500 °C and 600 °C. X-ray diffractometry shows that samples grown in this temperature range are epitaxial and pure-phase. UV-VIS absorption spectra show a consistent bandgap of 2.5 ± 0.03 eV for all growth temperatures. A small tail in the UV-VIS absorption spectra just below the bandgap extends down to 2.2 eV, indicating some electronic states within the bandgap. The bandgap was confirmed via CL measurements, where a bandgap of 2.46 ± 0.01 eV was obtained for samples at growth temperatures of 550 °C and 600 °C. To our knowledge, this report is the first measured value of electronic band and defect structure for epitaxial BiFeO$_3$ films and confirms theoretical predictions.

Thursday, March 13, 2008 2:30PM - 5:30PM –
Session W39 GSNP: Focus Session: Jamming II: Packing and Force Networks

Morial Convention Center 231
2:30PM W39.00001 A phase diagram for jammed matter reveals the nature of the random loose and random close packing of spheres . PING WANG, CHAOMING SONG, HERMAN A. MAKSE, Levich Institute and Department of Physics, City College of New York — We employ statistical mechanics of jammed matter to demonstrate the phase diagram of all possible jammed configurations of frictional and frictionless granular packings. This provides a statistical definition of RLP and RCP, predicts their density values in close agreement with simulations, and establishes the concomitant equations of state relating observables such as the coordination number, z, entropy, S, and volume fraction, φ. We show that the RCP state is not a unique point in the phase space but extends along a line of zero compactivity, a temperature-like variable, predicted to be at a constant \( \eta_{RCP} = 0.634 \), but with different z. The lowest density of RLP appears as a line of infinite compactivity parameterized by z, ending at the minimum possible density theoretically predicted to be \( \Phi_{RLP} = 0.543 \). The nature of the disorder of the packings is statistically characterized by the entropy which is shown to be larger in the random loose case than in the random close case.

2:42PM W39.00002 Random loose packing of rough spheres1 . GREG FARRELL, MICHAEL MARTINI, NARAYAN MENON, Dept of Physics, UMass Amherst — We report experiments in which random loose packings of spheres are created by sequential deposition of monodisperse (3.18 ± 0.05mm) PMMA beads of high sphericity in a fluid. The deposition speed is controlled by varying the relative densities of the spheres and the fluid, as well as by varying fluid viscosity. As in the work of Onoda and Liniger, we find that the volume fraction of the sediment asymptotically approaches a lower limit as we approach neutral buoyancy. However, we find that deposition in increasingly viscous fluids has the same effect. We also study the effect on the packing of controlled chemical roughening of the surface of the spheres. The volume fractions attained can be significantly lower than the often-quoted volume fraction of 0.555 for random loose packing. Thus there is no unique volume fraction for the random loose packing of spheres; the measured volume fraction, even in the limit of slow deposition dynamics is determined by particle surface properties.

3:06PM W39.00004 Analysis of Configurational Entropy in Jammed Granular Matter . CHRISTOPHER BRISCOE, CCNY - Levich Institute, PING WANG, CHAOMING SONG, HERMAN MAKSE — Energy fluctuations in jammed granular matter are negligible and cannot control the statistical mechanics. It is of interest to explore volume fluctuations in an effort to describe the statistical mechanics of jammed matter, originally proposed by Edwards. Current studies have introduced the concept of a theoretical phase diagram for jammed matter, providing plausible statistical explanations for the RCP and RLP states, along with intermediate jammed states, as a function of coordination number, z, friction coefficient \( \mu \), and volume fraction, \( \phi \). Entropy can be derived from this theoretical framework by means of a Hamiltonian, with energy and temperature replaced by volume, W, and compactivity, X, where X is an analogue of temperature. Our present efforts are to calculate the Shannon entropy of jammed granular packings along various paths of the phase diagram, resulting in an extensive entropy density, and X, as a function of \( \phi \), providing a new equation of state for jammed granular matter.

3:18PM W39.00005 Jamming of Frictional Spheres . ABDULLAH CAKIR, LEONARDO SILBERT, Southern Illinois University — Packings of monodisperse, frictional spheres are studied for a wide range in particle friction coefficient on approach to the jamming transition — the point where the packing loses mechanical stability. In particular, we focus on dynamical properties through the study of the vibrational normal modes. The dynamical matrix includes terms that take into account the rotational degrees of freedom due to non-central forces in the presence of friction. The influence of friction on the normal mode frequencies and particle polarization vectors are examined. Distinct from frictionless systems, for finite friction, the normal modes now allow for particle rotations.

3:30PM W39.00006 Hard Discs on the Hyperbolic Plane . CARL MODES, RANDALL KAMIEN, University of Pennsylvania — We examine a simple hard disc fluid with no long range interactions on the two dimensional space of constant negative Gaussian curvature, the hyperbolic plane. This geometry provides a natural mechanism by which global crystalline order is prohibited, allowing us to construct a tractable model of disordered monodisperse hard discs. We extend free area theory and the virial expansion to this regime, deriving the equation of state for the system, and compare its predictions with simulation near an isostatic packing in the curved space.

3:42PM W39.00007 Random subcubes as a toy model for constraint satisfaction problems . THIERRY MORA, Princeton Univ, LENKA ZDEBOROVA, LPTMS, Univ. Paris-Sud — abstract-Many hard combinatorial problems, such as Random Satisfiability, have been shown to reproduce some nontrivial properties of glassy materials. In particular, it has been proved that the configurational landscapes of the hardest problems are made of many disconnected ergodic components, leading to rich phase diagrams. Here we present an exactly solvable random-subcube model inspired by the structure of hard constraint satisfaction and optimization problems. Our model reproduces the structure of the solution space of the satisfiability and coloring problems, and undergoes the same phase transitions. Distance properties, and their relation to ergodicity, are studied. The model can also be generalized to define a continuous energy landscape useful for studying several aspects of glassy dynamics.

3:54PM W39.00008 Random Packing of Platonic Solids . TABER HERSUM, MARTIN-D. LACASSE, HUBERT KING, ExxonMobil Research & Engineering Company — While a large amount of literature has been devoted to the packing of spheres, very little is known about the packing of regular polyhedra, such as platonic solids. This presentation will describe numerical work on the packing of model systems in which mono-disperse tetrahedra, cubes, dodecahedra, and icosahedra are randomly packed. Energy fluctuations in jammed granular matter are mapped to random satisfiability and coloring problems, and undergoes the same phase transitions. Distance properties, and their relation to ergodicity, are studied. The point where the packing loses mechanical stability. In particular, we focus on dynamical properties through the study of the vibrational normal modes. The dynamical matrix includes terms that take into account the rotational degrees of freedom due to non-central forces in the presence of friction. The influence of friction on the normal mode frequencies and particle polarization vectors are examined. Distinct from frictionless systems, for finite friction, the normal modes now allow for particle rotations.

4:08PM W39.00009 Experiments on Random Packings of Tetrahedrons1 . ALEXANDER JAOSHLIVI, PAUL CHAISKIN, New York University — We have performed experiments related to the random packing of tetrahedral. The main experiments are MRI scans of tetrahedral molecule from which we determine their positions and orientations. We have done a direct analysis of the dice packing. The dice differ from mathematical tetrahedral in having slightly rounded vertices and edges. We have performed a best fit to each die to a perfect tetrahedral and then relaxed the packing to reduce the resulting overlaps. Analyzed data for the dice, the relaxed tetrahedra and simulations include the packing density, the orientational and spatial correlation functions, the average coordination number as well as the distribution of point to face, edge to edge and edge to face contacts. We also study the boundary effects from the walls and the distribution of constraints per particle. Our measurements indicate that random packed tetrahedral have a very small spatial or orientational correlation length. They are more random, that is with smaller and shorter range correlations than what has been found for spheres, or ellipsoids.

1 NSF, DMR0604295.
Local pressure distributions in the force network ensemble for granular media, BRIAN TIGHE, Universiteit Leiden — We present an analytic calculation of the probability distribution of pressure on individual grains in a static granular packing. We maximize entropy within an ensemble of all possible force networks on a fixed contact network, which incorporates force balance on each grain. Similar to energy in the microcanonical ensemble, the average pressure in each configuration is fixed. Subject to this global constraint alone, entropy maximization would yield a pressure distribution with an exponential tail. We demonstrate that, as a direct consequence of local force balance, there exists an additional global conserved quantity. Maximizing entropy while also respecting this new conserved quantity, we find a pressure distribution that, in frictionless packings, grows as a power law for small pressures and decays with a Gaussian tail. The form of the distribution is confirmed by numerics. As we increase the coefficient of friction, the tail approaches an exponential.

Using MR Elastography to Image Force Chains in a Quasi-Static Granular Assembly, L. SANFRATELLO, S.A. ALTOBELLI, NMR, R.P. BEHRINGER, Duke University, E. FUKUSHIMA, ABQMR — Questions about the internal structure of dense granular assemblies remain unanswered for lack of 3D experimental data. It is known from 2D observations and from the boundaries of 3D systems that non-uniform stresses are present on container boundaries as well as at the bottom of granular piles. These forces are seen in 2D to be distributed by force chains, where most of the stress is transmitted through a small number of chains with much of the assembly transmitting little or none of the force. However, force chains have yet to be fully visualized in 3D. We propose a variation of magnetic resonance elastography (MRE) to image 3D force chains within a densely packed granular assembly. MRE is an MRI technique whereby small periodic displacements within an elastic material can be measured. Multiple bipolar motion encoding gradients incorporated into a typical pulse sequence, and applied at the frequency of mechanical oscillations, are used to detect the displacements. We have verified our MRE technique using a gel (Perma-Gel). We now extend this method to image force chains within a 3D granular assembly of particles under stress, on top of which is superimposed a small-amplitude vibration. It is our hypothesis that significant coherent displacements will be found only along force chains while most particles will move randomly. Experimental results will be presented.

Abstract Contact Percolation in Dense Granular Flow, FUPING ZHOU, ExxonMobil Research and Engineering Company, DENIZ ERTAS, ExxonMobil Research and Engineering — Steady-state rheology of spheres are studied in the dense flow regime with three-dimensional molecular dynamics simulations in two different geometries: Simple shear flow and gravity-driven chute flow. The same set of constitutive equations, which are only a function of the local dimensionless strain rate, I, are found to characterize bulk macroscopic observables such as density, internal Coulomb coefficient and scaled velocity fluctuations in both cases. A transition has been identified at a finite (non-universal) value of I = Ic, corresponding to the percolation transition of the instantaneous contact network. For I < Ic, an infinite contact network spans the system. The flow dilutes and the internal Coulomb coefficient increases with increasing I. For I > Ic, the instantaneous contact network is broken into finite clusters. The system dilutes further with increasing I while the internal Coulomb coefficient becomes independent of I, reaching a maximum tilt angle for steady chute flow. Scaled velocity fluctuations exhibit power-law dependence on I on both sides of Ic, with a minimum at the transition. The transition is distinct from the “jamming” transition at I = 0 associated with the rigidity percolation of the contact network.

Dynamics of the Granular Jamming Transition, MAHESH BANDI, Los Alamos National Laboratory, ANDRIAS LIBAL, Johns Hopkins University, MICHAEL RIVERA, ROBERT ECKE, Los Alamos National Laboratory — We experimentally study the force fluctuations felt by a probe disk as it is dragged through a two-dimensional bi-disperse system of randomly packed photo-elastic disks. The fluctuations are studied as a function of packing fraction where the system goes from an unjammed to a jammed state with increasing packing fraction. As the system approaches the Jamming Point, the fluctuations are expected to diverge and become increasingly intermittent. We will present preliminary results of the force fluctuations felt by the probe disk as measured by a force transducer and compare them with visual data as obtained from the force-chains formed by the photo-elastic disks.

Stick-Slip and Granular Force Networks, ROBERT BEHRINGER, PEIDONG YU, Duke University — We describe friction/failure experiments for a granular system consisting of photoelastic particles. The goal of the experiments is to provide a microscopic understanding of stick-slip friction for an object that is pulled across a granular material. The granular material consists of a photoelastic disks (biphasic distribution) that are confined to a vertically oriented channel. A slider that is rough at the grain scale is pulled across the upper surface of the material. The pulling is accomplished by a screw-driven platform that is connected to the slider by a spring. Photoelastic image data are acquired by a camera and light source that move with the platform. Non-periodic stick-slip occurs for the regime of parameters studied here. During a stick event, force builds up in a strong network of force chains in the granular material. When one or more of the chains break, a slip event occurs. Energy changes from these events are power-law distributed. Analysis of failure points and slip events yields the effective friction coefficients, which are broadly scattered. An alternative description involves modeling the force chain network as a collection of springs. Failure of one spring can lead to a cascade and hence the broad distribution of energy losses.

Supported by ARO grant W911NF-07-1-0131-00

Thursday, March 13, 2008 2:30PM - 5:30PM —
Session W40 DBP GSNP: Focus Session: Networks, Regulation, and Pathways in Cell Biology

2:30PM W40.00001 Metabolism and evolution: A comparative study of reconstructed genome-level metabolic networks, EIVIND ALMAAS, Lawrence Livermore Natl Lab — The availability of high-quality annotations of sequenced genomes has made it possible to generate organism-specific comprehensive maps of cellular metabolism. Currently, more than twenty such metabolic reconstructions are publicly available, with the majority focused on bacteria. A typical metabolic reconstruction for a bacterium results in a complex network containing hundreds of metabolites (nodes) and reactions (links), while some even contain more than a thousand. The constrain-based optimization approach of flux-balance analysis (FBA) is used to investigate the functional characteristics of such large-scale metabolic networks, making it possible to estimate an organism’s growth behavior in a wide variety of nutrient environments, as well as its robustness to gene loss. We have recently completed the genome-level metabolic reconstruction of Yersinia pseudotuberculosis, as well as the three Yersinia pestis biovars, Antiqua, Mediaevalis, and Orientalis. While Y. pseudotuberculosis typically only causes fever and abdominal pain that can mimic appendicitis, the evolutionary closely related Y. pestis strains are the aetiological agents of the bubonic plague. In this presentation, I will discuss our results and conclusions from a comparative study on the evolution of metabolic function in the four Yersiniae networks using FBA and related techniques, and I will give particular focus to the interplay between metabolic network topology and evolutionary flexibility.

Work was performed under the auspices of the DoE by LLNL under Contract DE-AC52-07NA27344, and supported by LDRD grant 06-ERD-061.
3:06PM W40.00002 Level architecture in genetic regulatory networks and the role of microR-NAs, J. M. SCHWARZ, Physics Department, Syracuse University — It is well known that genes that code for proteins regulate the expression of each other through protein-mediated interactions. With the discovery of microRNAs (miRNAs), it has been conjectured that there are many such regulatory miRNAs in the cell that are never transcribed into proteins but are important for regulation and, hence, could explain the nature of the non-coding (or junk) DNA. Furthermore, miRNAs are highly conserved molecules. So, just as genes that code for proteins form regulatory networks, we conjecture that miRNAs form a higher-level regulatory network amongst themselves as mediated by the genes-coding-for-proteins regulatory network to form a complex organism. We investigate this conjecture within the framework of random Boolean networks where the two-level architecture is modelled via two coupled random Boolean networks with one network taking precedence over the other for various input/output values. Aspects of the evolution of the lower-level network will also be addressed.

3:18PM W40.00003 Tailoring the metabolism against mutations, NATALI GULBAHCE, Northeastern University, ADILSON E. MOTTER, Northwestern University, EIVIND ALMAAS, Lawrence Livermore National Laboratory, ALBERT LASZLO BARABASI, Northeastern University — In the post-genomic era, organisms can be modelled at the whole-cell level in silico via steady state methods to describe their metabolic capabilities. We use two such methods, Flux Balance Analysis and Minimization of Metabolic Adjustment to explore the behavior of cells (of E. coli and S. cerevisiae) after severe mutations. We propose experimentally feasible ways of modifying the underlying biochemical reaction network of a mutant cell such that cell functionality, in particular growth rate, is significantly improved.

3:30PM W40.00004 Form, Function, and Evolvability in Biological Networks, ANDREW MUGLER, Physics Dept, Columbia University, EYTZ ZIV, College of Physicians and Surgeons, Columbia University, ILYA NEMENMAN, CCS-3/CNLS, Los Alamos National Laboratory, CHRIS H. WIGGINS, Dept of Applied Physics & Applied Math/C2B2, Columbia University — A driving problem in systems biology for several years has been exploring the extent to which the topology of a small biological network constrains or guides its function. The absence of such constraint would allow a given network to evolve without rewiring its underlying form. We introduce a quantitative measure of this evolvability that does not rely on pre-defining the preferred function of a given topology. We then study the stochastic description of the experimental setup of Guet [1], treating chemical inducers as functional inputs and the expression of a reporter gene as the functional output. We take an information-theoretic approach, allowing the system to set parameters that optimize signal processing ability, thus enumerating the highest-fidelity functions. We find that, while all networks studied are highly evolvable by our measure—meaning that the function has little dependence on location in parameter space—the evolvability is correlated with individual topological features. Certain topological attributes, then, are shown (with statistical significance) to convey evolvability to biological networks. [1] C. C. Guet et al., Science 296, 1466 (2002).

3:42PM W40.00005 Noisy out of necessity: Probabilistic behavior during cellular differentiation, GUROL SUEL, UT Southwestern — Diverse organisms ranging from bacteria to mammalian stem cells undergo pluripotent differentiation where a single cell can commit to one out of several cell fates. How do underlying genetic circuits comprised of interactions between genes and proteins allow cells to "choose" a specific cell fate and execute the appropriate differentiation program? To address this question we investigate a simple bacterial differentiation system utilizing mathematical modeling and quantitative single cell measurements. In particular we are interested in elucidating the role of circuit dynamics and stochastic behavior in cellular differentiation.

4:18PM W40.00006 Analysis of temperature-dependent changes in the metabolism of Yersinia pestis,1 ALI NAVID, EIVIND ALMAAS, Lawrence Livermore National Laboratory — The gram-negative bacterium Yersinia pestis is the aetiological agent of bubonic plague, a zoonotic infection that occurs through the bite of a flea. It has long been known that Y. pestis has different metabolic needs upon transition from the flea gut environment (26 °C) to that of a mammalian host (37 °C). To study this and other outstanding questions about metabolic function of Y. pestis, we used the available genomic, biochemical and physiological data to develop a constraint-based flux balance model of metabolism in the avirulent 91001 strain (biovar Mediaevalis) of this organism. Utilizing two sets of whole-genome DNA microarray expression data, we examined the system level changes that occur when Y. pestis acclimates to temperature shifts. Our results point to fundamental changes in its oxidative metabolism of sugars and use of amino acids, in particular that of arginine. This behavior is indicative of an inefficient metabolism that could be caused by adaptation to life in a nutrient rich environment.

4:28PM W40.00007 Information processing in the E. coli Chemotaxis Network, LIN WANG, SIMA SETAVESHGAR, Department of Physics, Indiana University, Bloomington, IN — Biochemical signal transduction, broadly defined as the conversion of the concentration of an input signal to an output response, is the most basic level of biological information processing. The chemosensory pathway in bacterial chemotaxis is the best-characterized signal transduction network, and as such it provides an ideal system for probing the physical principles governing complex cellular signaling and response. Using an experimentally realistic stochastic implementation of the E. coli chemotaxis network and motor response, we investigate optimality of the chemotactic response in terms of input/output information transmission.

4:42PM W40.00008 Correlated Phenotypic Transitions to Competence in Bacterial Colonies, INBAL HECHT, Center for Theoretical Biological Physics, University of California, San Diego, ESHEL BEN-JACOB, School of Physics and Astronomy, Tel Aviv University, Israel, HERBERT LEVINE, Center for Theoretical Biological Physics, University of California, San Diego — Genetic competence is a phenotypic state of a bacterial cell in which it is capable of importing DNA, presumably to hasten its exploration of alternate genes in its quest for survival under stress. Recently, it was proposed that this transition is uncorrelated among different cells in the colony. Motivated by several discovered signaling mechanisms which create colony-level responses, we present a model for the influence of quorum-sensing signals on a colony of B. Subtilis cells during the transition to genetic competence. Coupling to the external signal creates an effective inhibitory mechanism, which results in anti-correlation between the cycles of adjacent cells. We show that this scenario is consistent with the specific experimental measurements, which fails to detect some underlying collective signaling mechanisms. Rather, we suggest other parameters that should be used to verify the role of a quorum-sensing signal. We also study the conditions under which phenotypic spatial patterns may emerge.

4:54PM W40.00009 On the Selection of Bistability in Genetic Regulatory Circuits, CHEOL-MIN GHIM, EIVIND ALMAAS, Lawrence Livermore National Laboratory, MICROBIAL SYSTEMS BIOLOGY TEAM — Bistability is a defining character of switching and memory devices. Many regulatory circuits observed in cellular reaction networks contain "bistability motifs" that endow a cell with efficient and reliable switching between different physiological modes of operation. One of the best characterized system, the lac operon in E. coli, has been shown to display a saddle-node bifurcation when induced by nonmetabolizable lactose analogue inducers, such as isopropylthio-β-D-galactoside (IPTG) and thio-methyl-galactoside (TMG). Motivated by the absence of bifurcation in the same system with its natural inducer, lactose, we studied the conditions for bistability and rationalized its fitness effects in the light of evolution. Stochastic simulations as well as mean-field approach confirm that history-dependent behavior as well as nongenetic inheritance, being realized by bistability motifs, may be beneficial in fluctuating environments.

1This project (06-ERD-061) was funded by the LDRD program at LLNL under the auspices of USDOE (contract # W-7405-ENG-48).
5:06PM W40.00010 Mutual information in random Boolean models of regulatory networks

JOSHUA SOCOLAR, Physics Dept. and Center for Systems Biology, Duke University. ANDRE RIBEIRO, Tampere University of Technology. BJORN SAMUELSSON, Lund University. JASON LLOYD-PRICE, STUART KAUFFMAN, University of Calgary — In a large, complex network of interacting elements, such as a genetic regulatory network within a cell, the average of the mutual information over all pairs of elements is a global measure of how well the system can coordinate its internal dynamics. We study the average pairwise mutual information I in random Boolean networks (RBNs) as a function of the distribution of Boolean rules implemented at each element, assuming that the links in the network are randomly placed. As the number N of network nodes approaches infinity, NI exhibits a discontinuity at parameter values corresponding to critical RBNs. For finite systems, NI peaks near the critical value, but slightly in the disordered regime for typical parameter variations. The source of high values of NI is the indirect correlations between pairs of elements from different long chains with a common starting point. The contribution from pairs that are directly linked approaches zero for critical networks and peaks deep in the disordered regime.

1Research supported by the National Science Foundation and the Alberta Informatics Circle of Research Excellence.

5:18PM W40.00011 Dynamical properties of structured Boolean networks

ANDREW POMERANCE, WOLFGANG LOSERT, MICHELLE GRIVAN, EDWARD OTT, University of Maryland, College Park — Boolean networks have been used since the 60s as a model for genetic control networks. In this model, each node takes on the value 0 or 1, modeling whether a gene is expressed or not, and updates at each time step according to a function of the value of its inputs. Random boolean networks (RBNs), where each node is randomly connected to other nodes and the function governing the dynamics is initially randomly generated, have been particularly well-studied. In particular, since these are deterministic, finite systems, the system must eventually settle into a periodic or fixed point attractor. A key question has been the scaling of the number of attractors with system size. In this talk we present results on how network structure effects the behavior of Boolean networks with randomly assigned dynamical rules. For example, we show that the number of attractors is dramatically increased by the addition of community structure to the network from the baseline RBN count with the same number of nodes. Furthermore, imposing bipartite structure on the network has little effect on the number of attractors.

Friday, March 14, 2008 8:00AM - 9:48AM –
Session X3 DCMP: Interface Phenomena in Oxides – Morial Convention Center RO2 - RO3

8:00AM X3.00001 2D Superconductivity at the LaAlO3/SrTiO3 interface

NICOLAS REYREN, University of Geneva — In 2004 Ohtomo and Hwang [1] discovered that the interface between two insulating oxides, LaAlO3 and SrTiO3 (both band insulators), is metallic with a high mobility. This publication triggered a lot of work around the world (see for instance [2, 3]). We have studied the ground state of this system and discovered superconductivity [4]. The studied LaAlO3 samples are grown epitaxially by pulsed laser deposition on TiO2-terminated SrTiO3 substrates and are annealed in situ in oxygen. The superconducting properties in the LaAlO3/SrTiO3 heterostructures display signatures of 2D superconductivity and agree with the Beresinskii-Kosterlitz-Thouless (BKT) predictions. However, for low currents, IV curves show some deviation from the expected behavior of a perfect infinite 2D system. These deviations are attributed to the finite lateral size of the measured path. Experiments to probe this size effect have been done to check this interpretation.


8:36AM X3.00002 Magnetic effects at the interface between nonmagnetic oxides

ALEXANDER BRINKMAN, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — The electronic reconstruction at the interface between two insulating oxides can give rise to a highly conductive interface. In analogy to this remarkable interface-induced conductivity we show how, additionally, magnetic effects can be induced at the interface between the otherwise nonmagnetic insulating perovskites SrTiO3 and LaAlO3 [1]. A large negative magnetoresistance, up to 50% at 50 mK, of the interface is found together with a logarithmic temperature dependence of the sheet resistance. These magnetic effects only appear in samples that have been grown under conditions that minimize the incorporation of oxygen vacancies. It is suggested that the interface electronic reconstruction induces localized magnetic moments in the SrTiO3 that interact with the conduction electrons. At low temperatures, the sheet resistance reveals magnetic hysteresis with a long relaxation time scale. The conducting oxide interface now provides a versatile system to induce and manipulate magnetic moments in otherwise nonmagnetic materials.


9:12AM X3.00003 Transport properties observed at hetero-interfaces of LaAlO3 on SrTiO3; intrinsic or extrinsic interface effect?

GERTJAN KOSTER1, GLAM, Stanford University — We have made very thin films of LaAlO3 on TiO2 terminated SrTiO3 and have measured the properties of the resulting interface in various ways. Transport measurements show a sheet carrier density of 10^{16} cm^{-2} and a mobility around 10^{3} cm^{2} V^{-1} s^{-1}. In situ UPS results indicate that oxygen vacancies play an important role in the creation of the charge carriers and that these vacancies are introduced by the pulsed laser deposition process used to make the hetero-interfaces [1]. Our results explain for the first time the origin of the large sheet carrier densities and high mobility observed previously [2]. XAS and spectroscopic ellipsometry [3] measurements confirm the existence of (oxygen) defects in the SrTiO3. Simple model calculations confirm the plausibility of having defects at the origin of charge carriers while still maintaining a high mobility. By means of annealing experiments in atomic oxygen we try to answer the question whether an intrinsically doped interface does indeed exist at lower carrier concentrations [2]. Due to its reactive nature (i.e., binding energy in an oxygen molecule is about 5 eV), atomic oxygen will have much more power to eliminate any oxygen vacancies compared to conventional annealing methods.


Work presented was done at Stanford University.

Friday, March 14, 2008 8:00AM - 11:00AM –
Session X4 DCMP GQI: Approaching Quantum Limits in Optomechanical Systems – Morial Convention Center 206
Sensing nanomechanical motion with a microwave cavity interferometer.

CINDY REGAL, JILA: NIST and the University of Colorado, Boulder — Optomechanical and electromechanical systems utilizing micro and nanomechanical oscillators offer a promising route towards manipulation of macroscopic objects at the quantum level. In this talk I present experiments that use principles of popular optomechanical systems yet employ light at microwave frequencies. Operating at microwave frequencies allows us to also harness technology associated with electromechanical systems, such as very light nanoscale mechanical objects and on-chip circuit elements compatible with a dilution refrigerator environment. Specifically, in our work we embed a nanomechanical flexural resonator inside a superconducting transmission-line microwave cavity, where the mechanical resonator’s position couples to the cavity capacitance and thus to the resonant frequency of the cavity. With our device we realize near state-of-the-art force sensitivity ($3 \times 10^{-19} \text{N}$/Hz) and thus add to only a handful of techniques able to measure thermomechanical motion at 10’s of miliKelvin temperatures. Our current measurements achieve a promising total displacement uncertainty at 140 times the quantum limit and a measurement imprecision as low as 30 times the quantum limit, as well as elucidate the important steps that will be required to progress towards the full quantum limit of displacement detection with this new system.

Strong dispersive coupling between a micromechanical oscillator and a high finesse optical cavity.

JACK HARRIS, Departments of Physics and Applied Physics, Yale University, New Haven, CT — Very sensitive mechanical detectors spanning roughly seventeen orders of magnitude in size are rapidly approaching a regime in which either the mechanical device itself or its readout should demonstrate quantum behavior. One of the main technical barriers to actually reaching this regime has been the difficulty of integrating ultrasensitive micromechanical devices with high-finesse optical cavities. Recently we have developed a robust means for addressing this issue, and have integrated a 50 nm-thick membrane (with a quality factor $>1,000,000$) into an optical cavity with a finesse $\sim 20,000$. Although the membrane is nearly transparent, it couples to the optical cavity dispersive. This coupling is strong enough to enable coherent control of the mechanical resonance of the membrane. We will describe our experimental results, as well as our progress towards observing quantum effects in this system.

Cavity Assisted Sideband Cooling of Mechanical Motion.

FLORIAN MARQUARDT, Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Ludwig-Maximilians University Munich, Germany — This talk will provide a pedagogical introduction to the theoretical ideas that form the basis for cooling a mechanical cantilever using light-induced forces. During recent years, these concepts have been realized in a series of experiments by various groups, that have demonstrated impressive progress in cooling. Several of them will be discussed in the following talks of this session. Ultimately, this line of research may lead to the quantum-mechanical ground state of the center-of-mass motion of objects composed of many billions of atoms. A common ingredient is the use of an optical cavity to resonantly enhance the radiation pressure force affecting the motion of the cantilever. I will start by reviewing the classical description of how a time-retarded force leads to enhanced friction and thus cooling. Then I will present a fully quantum-mechanical description, that takes into account the opposing effect of the photon shot noise [F. Marquardt, J. P. Chen, A. A. Clerk and S. M. Girvin, Phys. Rev. Lett. 99, 093902 (2007); see also I. Wilson-Rae, N. Nooshi, W. Zwerger and T. J. Kippenberg, Phys. Rev. Lett. 99, 093901 (2007)]. This theory yields a quantum-limit for the reachable photon number that can be made arbitrarily small, provided a high-finesse cavity is combined with a high-frequency mirror (the “resolved sideband limit,” analogous to ion cooling). Various different ways of experimentally measuring the photon number will be mentioned. Finally, I will briefly give an outlook regarding the possibilities for quantum-coherent experiments that will open up once the ground state has been reached. This talk primarily reports joint work with A. Clerk, J. P. Chen, and S. Girvin.

Laser Cooling of Gram Scale Objects.

THOMAS CORBITT, Massachusetts Institute of Technology — Laser cooling of macroscopic mechanical oscillators is a rapidly growing field with applications in high precision measurements, gravitational wave detectors, and exploration of the classical-quantum transition. Here I will describe a series of cooling experiments, which are inspired by gravitational wave detectors, to trap and cool gram scale mirror oscillators. To approach quantum limits of oscillators with such a high mass requires the use of a variety of cooling techniques. The techniques employ non-mechanical forces both to trap the mirror by increasing its effective mechanical resonant frequency, and to cool the mirror by damping its motion within the trap. The non-mechanical forces are created from either radiation pressure in a detuned optical resonator, or from electronic feedback forces in an active servo. As the experiments approach the quantum regime, an assortment of non-classical behavior and effects should become evident, such as quantum radiation pressure noise, and squeezing and entanglement of the light and mirror states. I will discuss the prospects for observation of these effects, in light of current performance and expected upgrades.

Towards experimental optomechanical entanglement between a movable mirror and a cavity field.

MARKUS ASPELMEYER, Austrian Academy of Sciences — The quantum regime of mechanical systems offers fascinating new possibilities for both applied and fundamental physics. Quantum optics provides a well-developed tool box to help entering and controlling this regime as is evidenced by the recent successes in laser-cooling of micromirrors that promise cooling capabilities to the mechanical quantum ground state. I will start by reviewing the classical description of how a time-retarded force leads to enhanced friction and thus cooling. Then I will describe a series of cooling experiments, which are inspired by gravitational wave detectors, to trap and cool gram scale mirror oscillators. To approach quantum limits of oscillators with such a high mass requires the use of a variety of cooling techniques. The techniques employ non-mechanical forces both to trap the mirror by increasing its effective mechanical resonant frequency, and to cool the mirror by damping its motion within the trap. The non-mechanical forces are created from either radiation pressure in a detuned optical resonator, or from electronic feedback forces in an active servo. As the experiments approach the quantum regime, an assortment of non-classical behavior and effects should become evident, such as quantum radiation pressure noise, and squeezing and entanglement of the light and mirror states. I will discuss the prospects for observation of these effects, in light of current performance and expected upgrades.

THURSDAY, MARCH 13, 2008 8:00AM - 11:00AM —
Session X4 DCMP: Superconducting Sources of THz-Radiation

8:00AM X4.00001 Sensing nanomechanical motion with a microwave cavity interferometer.

CINDY REGAL, JILA: NIST and the University of Colorado, Boulder — Optomechanical and electromechanical systems utilizing micro and nanomechanical oscillators offer a promising route towards manipulation of macroscopic objects at the quantum level. In this talk I present experiments that use principles of popular optomechanical systems yet employ light at microwave frequencies. Operating at microwave frequencies allows us to also harness technology associated with electromechanical systems, such as very light nanoscale mechanical objects and on-chip circuit elements compatible with a dilution refrigerator environment. Specifically, in our work we embed a nanomechanical flexural resonator inside a superconducting transmission-line microwave cavity, where the mechanical resonator’s position couples to the cavity capacitance and thus to the resonant frequency of the cavity. With our device we realize near state-of-the-art force sensitivity ($3 \times 10^{-19} \text{N}$/Hz) and thus add to only a handful of techniques able to measure thermomechanical motion at 10’s of miliKelvin temperatures. Our current measurements achieve a promising total displacement uncertainty at 140 times the quantum limit and a measurement imprecision as low as 30 times the quantum limit, as well as elucidate the important steps that will be required to progress towards the full quantum limit of displacement detection with this new system.

8:36AM X4.00002 Strong dispersive coupling between a micromechanical oscillator and a high finesse optical cavity.

JACK HARRIS, Departments of Physics and Applied Physics, Yale University, New Haven, CT — Very sensitive mechanical detectors spanning roughly seventeen orders of magnitude in size are rapidly approaching a regime in which either the mechanical device itself or its readout should demonstrate quantum behavior. One of the main technical barriers to actually reaching this regime has been the difficulty of integrating ultrasensitive micromechanical devices with high-finesse optical cavities. Recently we have developed a robust means for addressing this issue, and have integrated a 50 nm-thick membrane (with a quality factor $>1,000,000$) into an optical cavity with a finesse $\sim 20,000$. Although the membrane is nearly transparent, it couples to the optical cavity dispersive. This coupling is strong enough to enable coherent control of the mechanical resonance of the membrane. We will describe our experimental results, as well as our progress towards observing quantum effects in this system.

9:12AM X4.00003 Cavity Assisted Sideband Cooling of Mechanical Motion.

FLORIAN MARQUARDT, Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Ludwig-Maximilians University Munich, Germany — This talk will provide a pedagogical introduction to the theoretical ideas that form the basis for cooling a mechanical cantilever using light-induced forces. During recent years, these concepts have been realized in a series of experiments by various groups, that have demonstrated impressive progress in cooling. Several of them will be discussed in the following talks of this session. Ultimately, this line of research may lead to the quantum-mechanical ground state of the center-of-mass motion of objects composed of many billions of atoms. A common ingredient is the use of an optical cavity to resonantly enhance the radiation pressure force affecting the motion of the cantilever. I will start by reviewing the classical description of how a time-retarded force leads to enhanced friction and thus cooling. Then I will present a fully quantum-mechanical description, that takes into account the opposing effect of the photon shot noise [F. Marquardt, J. P. Chen, A. A. Clerk and S. M. Girvin, Phys. Rev. Lett. 99, 093902 (2007); see also I. Wilson-Rae, N. Nooshi, W. Zwerger and T. J. Kippenberg, Phys. Rev. Lett. 99, 093901 (2007)]. This theory yields a quantum-limit for the reachable photon number that can be made arbitrarily small, provided a high-finesse cavity is combined with a high-frequency mirror (the “resolved sideband limit,” analogous to ion cooling). Various different ways of experimentally measuring the photon number will be mentioned. Finally, I will briefly give an outlook regarding the possibilities for quantum-coherent experiments that will open up once the ground state has been reached. This talk primarily reports joint work with A. Clerk, J. P. Chen, and S. Girvin.

9:48AM X4.00004 Laser Cooling of Gram Scale Objects.

THOMAS CORBITT, Massachusetts Institute of Technology — Laser cooling of macroscopic mechanical oscillators is a rapidly growing field with applications in high precision measurements, gravitational wave detectors, and exploration of the classical-quantum transition. Here I will describe a series of cooling experiments, which are inspired by gravitational wave detectors, to trap and cool gram scale mirror oscillators. To approach quantum limits of oscillators with such a high mass requires the use of a variety of cooling techniques. The techniques employ non-mechanical forces both to trap the mirror by increasing its effective mechanical resonant frequency, and to cool the mirror by damping its motion within the trap. The non-mechanical forces are created from either radiation pressure in a detuned optical resonator, or from electronic feedback forces in an active servo. As the experiments approach the quantum regime, an assortment of non-classical behavior and effects should become evident, such as quantum radiation pressure noise, and squeezing and entanglement of the light and mirror states. I will discuss the prospects for observation of these effects, in light of current performance and expected upgrades.

10:24AM X4.00005 Towards experimental optomechanical entanglement between a movable mirror and a cavity field.

MARKUS ASPELMEYER, Austrian Academy of Sciences — The quantum regime of mechanical systems offers fascinating new possibilities for both applied and fundamental physics. Quantum optics provides a well-developed tool box to help entering and controlling this regime as is evidenced by the recent successes in laser-cooling of micromirrors that promise cooling capabilities to the mechanical quantum ground state. I will discuss the prospects and challenges to generate (opto-mechanical) quantum entanglement, which is an important resource for quantum information processing and is also at the heart of Schrödinger’s “cat paradox.”
8:36 AM X5.00002 Emission of Coherent THz-Radiation from Superconductors. ULRICH WELP, Argonne National Laboratory — Josephson junctions naturally convert dc-voltages into high-frequency electromagnetic radiation, with 1 mV corresponding to 0.483 THz, and many such junctions emitting in phase at the same frequency can produce useful emission power. Stacks of junctions with unsurpassed packing density occur naturally in the layered high temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$, in which the superconducting CuO$_2$-layers are coupled through the intrinsic Josephson effect. However, achieving synchronization of the high-frequency oscillations of all the junctions in the stack has so far been a major challenge. We demonstrate that coherent continuous-wave THz-radiation of sizable power can be extracted from intrinsic Josephson junctions in the layered high-temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_8$. In analogy to a laser cavity, the excitation of an electromagnetic cavity resonance inside the sample generates a macroscopic coherent state in which a large number of junctions are synchronized to oscillate in phase. The emission power is found to increase as the square of the number of junctions reaching values of 0.5 μW at frequencies up to 0.85 THz. The available power is potentially much larger, as there is evidence that 20 μW of power are pumped into the observed THz cavity resonance. The emission persists up to temperatures of ~50 K. Emission does not require the application of a magnetic field, significantly simplifying the design of superconducting THz-sources. In fact, a single applied D.C. current leads to the efficient excitation of continuous coherent THz-radiation. This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357 – Basic Energy Sciences, the Japanese Ministry of Education, Culture, Sports, Science and Technology, and the Turkish TUBITAK under Project No. 106T053. In collaboration with L. Ozuyer, A. E. Koshelev, C. Kunter, N. Gopalasmi, Q. Li, M. Tachiki, K. Kadowaki, T. Yamamoto, H. Minami, H. Yamaguchi, T. Tachiki, K. E. Gray, W.-K. Kwok.

9:12 AM X5.00003 Radiation Due to Josephson Oscillations in Layered Superconductors. LEV BULAEVSKII, Los Alamos National Laboratory — The power of direct tunable radiation into free space induced by Josephson oscillations in intrinsic Josephson junctions of highly anisotropic layered superconductors is derived. The super-radiation regime in a current biased crystal is considered when no dc magnetic field is applied. It is assumed that crystal is cut in the form of thin plate parallel to the ac-plane with the thickness of several microns along the a-axis and length of several hundreds microns along the c-axis. At large number of intrinsic junctions oscillations in such BSCCO crystal are synchronized providing high radiation power proportional to squared number of junctions and high efficiency up to 1/3 in the THz frequency range. The radiation correction to the current-voltage characteristic in this regime depends only on crystal shape. When the ac-edge of such a crystal is irradiated by external electromagnetic wave, radiation from both ac-edges of the crystal is enhanced (stimulated radiation) at higher-current part of the Shapiro step. The main part of external radiation is in the direction opposite to incident wave. This effect of stimulated radiation may be used for amplification of electromagnetic waves. BSCCO crystal with modulated critical current and length several tens microns along the b-axis also provides high THz-radiation power from the ac-edges at discrete Josephson frequencies corresponding to the crystal thickness along the b-axis. In this case the effective power of radiation power in this case is due to Fiske resonances and super-radiation regime. The powerful almost standing electromagnetc wave is excited inside the crystal in the resonance. This wave is homogeneous across the layers meaning that the oscillations are synchronized in all junctions in the stack. In this situation the synchronization of radiation in different junctions is enforced by both super-radiation regime and similar critical current profile in all junctions of the crystal.

9:48 AM X5.00004 THz emission from a slice of high-Tc superconducting single crystal. HUABING WANG, National Institute for Materials Science, Tsukuba 3050047, Japan — Copper oxide superconductors possess intrinsically a layered crystalline structure in which the superconducting and non-superconducting layers interlace each other. Therefore the crystal itself consists of a number of superconducting junctions sequentially stacked along the c axis of the crystal, and these junctions are often referred to as intrinsic Josephson junctions (IJJs). In the case of Bi$_2$Sr$_2$CaCu$_2$O$_8$+δ (BSCCO), each IJJ measures approximately 1.5 nm thick. Many groups have been exploring the possibilities to develop terahertz (THz) detectors and oscillators based on IJJs, due to their high collective plasma frequencies (up to THz region), the uniformity in junction properties, the easiness to make a large junction array, and the low loss at high frequencies. Some years ago, IJJs single out from inside a slice of BSCCO single crystal with a double-sided process, THz response was successfully observed as sharp Shapiro steps at frequencies up to 2.5 THz, and harmonic mixings were carried out with harmonic numbers as large as 90. Recently observed have been THz oscillations in various structures of BSCCO IJJs, which can be excited by dc bias, in-plane magnetic fields, or microwave irradiations at several gigahertz. Needless to say, for practical applications, it is necessary to synchroize the emissions from IJJs, couple the THz oscillations into a finite channels, guide them in a controllable way, monitor the frequencies and power levels, and preferably do the jobs using an integrated system. We have been making extensive efforts to explore these ideas, and will report our latest results at the meeting.

10:24 AM X5.00005 Mechanism of the terahertz wave emission from intrinsic Josephson junctions of Bi$_2$Sr$_2$CaCu$_2$O$_8$, MASASHI TACHIKI, The University of Tokyo — We propose a mechanism for the strong emission of terahertz wave recently observed in current-biased mesa-shaped Bi$_2$Sr$_2$CaCu$_2$O$_8$ single crystals at Argonne National Laboratory. When the mesa width is approximately equal to or larger than the phase coherence length (c-axis), an external current is applied along the c-axis of the crystal. The modulating current is designed to result in a resonance excitation of cavity-mode of the transverse Josephson plasma in the voltage state. When the oscillating electric and magnetic fields of the excited plasma wave propagate in the direction opposite to incident wave, this effect of stimulated radiation may be used for amplification of electromagnetic waves. BSCCO crystal with modulated critical current and length several tens microns along the b-axis also provides high THz-radiation power from the ac-edges at discrete Josephson frequencies corresponding to the crystal thickness along the b-axis. The available power is potentially much larger, as there is evidence of stimulated radiation in this case is due to Fiske resonances and super-radiation regime. The powerful almost standing electromagnetic wave is excited inside the crystal in the resonance. This wave is homogeneous across the layers meaning that the oscillations are synchronized in all junctions in the stack. In this situation the synchronization of radiation in different junctions is enforced by both super-radiation regime and similar critical current profile in all junctions of the crystal.
9:12AM X6.00003 Electron tunneling in epitaxial magnetic tunnel junctions

XIAOQUANG ZHANG, Oak Ridge National Laboratory — The remarkable progress in the performance of tunneling magnetoresistance (TMR) junctions using MgO as the barrier layer, has confirmed the theoretical prediction of a very high TMR ratio from first-principles calculations [1,2]. The theoretical prediction was based on the understanding of the band filtering effect by a class of barrier materials, including ZnSe, and even vacuum, in addition to MgO, along particular crystalline orientations. The combination of the preferential filtering for the electrons with the $\Delta_3$ symmetry by the barrier layer, and the presence of the $\Delta_3$ band only in the majority spin channel of Fe, FeCo and Co electrodes, results in the high TMR ratio previously believed only achievable with half-metallic electrodes. Here we show that the agreement between the experiment and the first-principles theory goes beyond the TMR. The effects of barrier thickness, interface resonance states, and quantum confinement calculated from the first-principles for MgO based magnetic tunnel junctions are compared with experimental data. In addition to excellent agreement for each case, additional insights are obtained from the first-principles calculations that are otherwise not directly available from the experiments. We also discuss other candidate materials for high TMR junctions.


3 This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.

9:48AM X6.00004 TMR-related effects in structures involving semiconductors

JEAN-MARIE GEORGE, Unité Mixte de Physique CNRS-Thales — The growth of semiconductor heterostructures incorporating ferromagnetic material is a challenge for today’s spintronics. We will report on GaMnAs/III-V and MnAs/III-V tunnel junctions that fulfill this condition. In the case of GaMnAs related junctions, the complexity of the transport mechanisms associated with spin-orbit coupled states make this material a powerful means for finding novel effects and provides new challenges for theoretical understandings. This includes tunnel magnetoresistance (TMR) across single and double barriers [1] and tunnel anisotropic magnetoresistance (TAMR). As an illustration, the resonant TAMR on a GaAs quantum well can be used as a probe of the GaMnAs valence band anisotropy [2]. In the case of MnAs, the necessary low temperature growth mode to avoid intermixing at the interfaces favors the insertion of As anti-site in the III-V spacer layer. We will show how the tunneling magnetoresistance is then modified and how the major role of the defects in the conduction can be taken into account. For this we have proposed an analytical model of spin-dependent resonant tunneling through a 3D assembly of localized states (spread out in energy and in space) in a barrier [3]. An inhomogeneous distribution of localized states leads to resonant tunneling magnetoresistance inversion and asymmetric bias dependence as evidenced with a set of experiments with MnAs/GaAs(7–10 nm)/MnAs tunnel junctions. By extension, we show the possibility of using such spectroscopic measurements to show the spin asymmetry of ferromagnetic electrodes sandwiching an inhomogeneous tunnel barrier.


10:24AM X6.00005 Influence of spin polarized current on superconductivity and spin transport in organic semiconductors

JAGADEESH MOODERA, MIT — Spin conserved tunneling from a ferromagnetic (FM) electrode through an insulating barrier with a superconductor as the spin detector, was discovered by Meservey and Teword three decades ago. This phenomenon of spin polarized tunneling has been successfully utilized to understand many aspects of magnetism and superconductivity. In recent years enormous success is seen in magnetic tunnel junctions both from the fundamental viewpoint as well as due to their application in information technology. In general, BCS superconductivity with Cooper pairs formed at the Fermi level with electrons of opposite spins is not compatible with ferromagnetism which have parallel spin configuration. The superconducting state can be influenced by injecting spin polarized current in a controlled manner by properly tailoring the interfacial transmissivity between a ferromagnet (F) and a superconductor (S), resulting in a large magnetoresistance (MR) of over 1100% for a F/I/S/F multilayer system (I - insulator) or even infinite MR can be achieved in epitaxial metallic systems. Due to the competition between ferromagnetism and superconductivity, the superconducting transition temperature ($T_C$) in the spin parallel configuration is shifted below that of the spin anti-parallel configuration. This $T_C$ shift can much larger than that predicted by theories. Oscillation in $T_C$ is also observed. The field is the spin transport properties in organic semiconductors (OSs), a least explored area. Because OSs are composed of mostly light elements (i.e. C, H, N, O) and thus have a weaker spin-orbit interaction, low hyperfine interactions, spin coherence lengths can be long in these materials. Large spin decay length was observed in amorphous Rubrene. Recent developments in electron spin polarized tunneling through ultrathin layers of the molecular organic semiconductors such as Alq3 and Rubrene will be discussed.

1 ONR, NSF and KIST-MIT project grants support the research.

Friday, March 14, 2008 8:00AM - 11:00AM – Session X7 DCOMP: Understanding Strongly Correlated Materials with Dynamical Mean Field Theory Methods Morial Convention Center R05

8:00AM X7.00001 Mott Transition, Antiferromagnetism, and d-wave Superconductivity in Two-Dimensional Organic Conductors and in Cuprates Using Cluster Dynamical Mean Field Theory

A.-M.S. TREMBLAY, Universite de Sherbrooke — The main features of the phase diagram of high-temperature superconducting cuprates are a Mott insulator at half-filling, a pseudogap at finite doping and, in the ground state, the competition between antiferromagnetism, d-wave superconductivity and possibly other inhomogeneous phases. In the layered organics of the $\kappa$-BEDT-T family, it is pressure instead of doping that is varied but the competing phases and the Mott insulating behavior are similar to the cuprates. Approaches that claim to explain d-wave superconductivity in the cuprates must also explain this phenomenon in all other related classes of compounds described by the Hubbard model. Using Cluster Dynamical Mean-Field theory, we show that the main features of both phase diagrams, cuprates and organics, can be understood from the one-band model with hopping parameters taken from band structure and interaction of the order of the bandwidth. We emphasize the case of the organics, studying the Mott transition, antiferromagnetism and superconductivity on the anisotropic triangular lattice. The Mott transition in the normal phase can be continuous or first order depending on the value of the frustrating hopping $t'/t$. A d-wave superconducting phase appears between an antiferromagnetic insulator and a metal for $t'/t = 0.3 - 0.7$, or between a nonmagnetic Mott insulator (spin liquid) and a metal for $t'/t \geq 0.8$, in agreement with experiments on layered organic conductors including $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$. These phases are separated by a strong first order transition. The phase diagram gives much insight into the mechanism for d-wave superconductivity and on the question of the glue.

1 In collaboration with B. Kyang. Supported by NSERC, CRC program, CFI, MEQ, CIFAR, FQRTN
we find a coupling between flow fluctuations in the gradient and vorticity directions. Using 2 and fluctuating flows.

in the wormlike micellar interior, direct measurement of the shear-induced nematic phase transition is reported. More recently we have used Rheo-NMR to
value, not only indicating the clear existence of shear bands, but also that they are associated with fluctuations, and sometimes, with molecular alignment. The
localized, often with resolution down to a few 10s of microns In the study of shear banding phenomena in wormlike micelles, Rheo-NMR has proven of especial
structure. Furthermore, through the use of orientation-dependent terms in the spin interactions, such as the nuclear quadrupole or dipolar interactions, NMR
also provides information about colloidal or molecular organisation and dynamics, under conditions of flow. In particular, NMR offers the possibility of measuring

University of Wellington — Rheo-NMR gives access to detailed information about the flow field generated by the device used to induce deformational flow. It

9:12AM X7.00003 Nodal/Antinodal Dichotomy and the Two Gaps of a Superconducting Doped Mott Insulator . MARCELLO CIVELLI, Institut Laue Langevin — Using Cellular Dynamical Mean Field Theory, implemented with exact diagonalization as impurity solver, we study the superconducting state of the hole-doped two-dimensional Hubbard model. We mainly focus on qualitative aspects which characterize the approach to the Mott transition. We will show that our formalism leads to a natural decomposition of the photoemission energy-gap into two components. A first gap, stemming from the anomalous self-energy, dominates near the nodes and decreases with decreasing doping. The second gap has an additional contribution from the normal self-energy, inherited from the normal-state pseudo-gap. It is dominant near the antinodes and increases as the Mott insulating phase is approached. This behavior of the one-particle gap is relevant in the light of recent experimental studies reporting the presence of two different energy scales in the nodal and antinodal regions of high-temperature superconductors.

9:48AM X7.00004 DCA study of magnetic mediated superconductivity in the Hubbard model1, MARK JARRELL2, University of Cincinnati — The Dynamical Cluster Approximation (DCA) with quantum Monte Carlo as a cluster solver is used to study pairing in the two dimensional Hubbard model. The DCA adds non-local corrections to dynamical mean field theory by mapping the lattice onto a self-consistently embedded periodic cluster. The qualitative features of the cuprate phase diagram are captured by the DCA with a 2x2 cluster, which provides a mean field solution of the model. With increasing cluster size, the results are found to converge and display a finite d-wave transition temperature, establishing the presence of superconductivity in the model. A decomposition of the pairing interaction into its cross channels reveals that pairing is mediated by S=1 spin fluctuations. A simple renormalized spin fluctuation model is found to capture many of the properties of pairing and the spectra, including the high-energy kink waterfall structure and the structure of the leading order parameter. However, it fails to capture realistic features including long-ranged hopping, phonons and the pseudogap. Phonons, in particular, are found to enhance the pairing interaction by enhancing antiferromagnetism. Despite this, superconductivity is suppressed by local (Holstein, Breathing and Buckling) phonon modes through the formation of polaron which dramatically reduce the particle mobility.

1This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:24AM X7.00005 DMFT calculations of materials properties using the continuous time QMC method1, CHRIS MARIANELLI, Lawrence Livermore National Laboratory — The combination of DFT with DMFT has proven to be an instrumental method for describing realistic strongly correlated electron systems. In essence, DMFT treats the strongly correlated electrons near the Fermi surface while DFT treats the electrons which are less correlated. DMFT effectively maps the intractable lattice many-body problem onto a tractable impurity many-body problem. The DMFT impurity problem must be solved using numerical methods or approximate analytical methods, and this is the bottleneck of the entire procedure. Continuous time QMC has recently emerged as a dominant method to solve the DMFT impurity problem. We present applications of DFT+DMFT(QTMC-atomic-limit) to the cobaltates and Pu. In Pu, a variety of physical properties are calculated such as the Photoemission spectra, magnetic susceptibility, and the heat capacity. These physical properties are probed as a function of temperature and volume, and compared with experimental measurements. Additionally, we demonstrate the effect of the full on-site exchange interaction on the physical observables. In the cobaltates, the Fermi surface and heat capacity are calculated for Na0.3CoO2. We demonstrate that the topology of the Fermi surface depends sensitively upon the bare Hamiltonian. It is shown that consistent agreement with heat capacity measurements and ARPES experiments can only be achieved if the ω0 satellite pockets are not present at the Fermi surface.

1Support from NSF DMR 0431350

Support from NSF DMR-0706379, OISE-0730290 and DOE CMSN DE-FG02-04ER46129
2Work in collaboration with A. Macridin, Th. Maier, D.J. Scalapino, E.Khatami, B. Moritz

Friday, March 14, 2008 8:00AM - 10:48AM –
Session X8 DFD: Focus Session: Wormlike Micellar Fluids and Vesicles Morial Convention Center R06

8:00AM X8.00001 Rheo-NMR of shear banded flow in wormlike micelles , PAUL CALLAGHAN, Victoria University of Wellington — Rheo-NMR gives access to detailed information about the flow field generated by the device used to induce deformational flow. It also provides information about colloidal or molecular organisation and dynamics, under conditions of flow. In particular, NMR offers the possibility of measuring nuclear spin relaxation times and molecular self-diffusion coefficients, sensitive respectively to molecular brownian motions and their restrictions due to local structure. Furthermore, through the use of orientation-dependent terms in the spin interactions, such as the quadrupole or dipolar interactions, NMR permits the measurement of molecular order parameters. When combined with imaging methods, NMR in principle allows such measurements to be spatially localized, often with resolution down to a few 10s of microns In the study of shear banding phenomena in wormlike micelles, Rheo-NMR has proven of especial value, not only indicating the clear existence of shear bands, but also that they are associated with fluctuations, and sometimes, with molecular alignment. The subtlety of the correspondence (or lack of correspondence) between birefringence effects and shear banded flow has also been revealed. Recent measurements of shear-banded flow under Couette flow of the micellar system 10% w/v cetylpyridinium chloride and sodium salicylate (CPyCl/NaSal) molar ratio 2:1 in 0.5 M NaCl in 1H2O, indicate that shear banding fluctuations are consistent with the shear stress fluctuations observed in rheological measurements. Furthermore we find a coupling between flow fluctuations in the gradient and vorticity directions. Using 2H NMR spectroscopy on a deuterated probe molecule (n-decane) in the wormlike micellar interior, direct measurement of the shear-induced nematic phase transition is reported. More recently we have used Rheo-NMR to investigate the flow and alignment properties of worm-like micelles formed by a 5% w/v solution of the BASF difunctional block copolymer non-ionic surfactant, Pluronic P105 in water along with 4.3% w/v 1-phenylethanol-d5. A variety of shear-banding and alignment behaviours are observed, along with both stable and fluctuating flows.
we observe a tracer depletion in the high-shear phase, which may be to high normal forces.

direction and a wavelength corresponding to smallest dimension of the channel. Finally we discuss the hypothesis of passive tracers: depending on their size,

obtained in Couette rheometers. Then we study the development of an instability at the interface between the two phases, with a wavevector in the vorticity

the so called shear banding regime. First we deduce the local rheology of the solution from these velocity profiles, in agreement with the macroscopic rheology

the flow is increased, the velocity profiles reveal first a Newtonian phase, then apparition of a dramatically lower viscosity second phase at the walls, which is

the solution, independently from the slippage at the wall, according to a method already validated on non-Newtonian polymer solutions. As the pressure driving

UMR CNRS-ESPCI Gulliver 7083 — We characterize by Particle Image Velocimetry the Poiseuille flow a semi-dilute solution of wormlike micelles (a CTAB and

7083, GUILLAUME DEGRE, LOF - UMR CNRS-ESPCI Gulliver 7083, PATRICK TABELING, MMN, UMR CNRS-ESPCI Gulliver 7083, ARMAND AJDARI, PCT,

JOSEPH GLADDEN, JOEL MOBLEY, Dept. of Physics and Astronomy, University of Mississippi — Wormlike micellar fluids have long been studied as a model

Newtonian fluid. The dynamic microstructure of the fluid gives rise to a rich diversity of hydrodynamic phenomena. Generally, these fluids are studied in a low concentration regime (0-20 mM of surfactant). In this talk, we will discuss recent rheological and acoustic measurements of highly concentrated wormlike micellar fluids with concentrations of 50 - 400 mM cetyltrimethylammonium bromide (CTAB) and 30 - 240 mM (respectively) sodium salicylate (NaSAL) in the temperature range of 22 - 45 Celsius. In 200 mM CTAB fluids, the activation energy, derived from stress relaxation time measurements, exhibit a discontinuous shift from about 60 kT below 33 Celsius to about 40 kT above. Speed of sound and acoustic attenuation measurements were obtained by a broadband Fourier spectroscopic method using ultrasonic waves between 2 and 8 MHz. Each of the concentrations measured exhibits an peak in the acoustic attenuation between 33 and 38 Celsius. The speed of sound increases monotonically over 22 - 40 Celsius, very similar to pure water in both magnitude and temperature dependence. Measurement attenuations as a function of acoustic power using high intensity focused ultrasound will also be discussed.

For TEA fractions greater than 30 mM. For TEA fractions greater than 55 mM, threadlike micelle structures are present. From the SANS data we

of tetraethylammonium perfluorooctylsulfonate (TEAFOS) and lithium perfluorooctylsulfonate (LiFOS) in water using small angle neutron scattering (SANS).

results from atomic force microscopy studies of the structure of such gels will be presented.

Results obtained from atomic force microscopy studies of the structure of such gels will be presented.

1 NSF
2 Corresponding Author

In contrast to ‘inert’ polymeric networks, wormlike micelles continuously break and reform leading to an additional relaxation mechanism and the name ‘living polymers’. Observations in both classes of entangled fluids have shown that steady and transient shearing flows of these solutions exhibit spatial inhomogeneities such as ‘shear-bands’ at sufficiently large applied strains. In the present work, we investigate the dynamical response of a class of two-species elastic network models which can capture, in a self-consistent manner, the creation and destruction of elastically-active network segments, as well as diffusive coupling between the microstructural conformations and the local state of stress in regions with large spatial gradients of local deformation. These models incorporate a discrete version of the micellar breakage and reforming dynamics originally proposed by Cates and capture, at least qualitatively, non-affine tube deformation and chain disentanglement. The ‘flow curves’ of stress and apparent shear rate resulting from an assumption of homogeneous deformation is non-monotonic and linear stability analysis shows that the region of non-monotonic response is unstable. Calculation of the full inhomogeneous flow field results in localized shear bands that grow linearly in extent across the gap as the apparent shear rate increases. Time-dependent calculations in step strain, large amplitude oscillatory shear (LAOS) and in start up of steady shear flow show that the velocity profile in the gap and the total stress measured at the bounding surfaces are coupled and evolve in a complex non-monotonic manner as the shear bands develop and propagate.

9:48AM X8.00006 Investigating the structures and phase behavior of anionic perfluorinated surfactant using SANS, GARFIELD WARREN, DOBRIN BOSSEV, Indiana University — We have examined the structures formed by mixtures of tetraethylammonium perfluorooctylsulfonate (TEAFOS) and lithium perfluorooctylsulfonate (LiFOS) in water using small angle neutron scattering (SANS). SANS is an ideal method to characterize the morphology of such soft materials because the characteristic length scale of the surfactant structures and the possibility to apply the contrast variation technique. Results were obtained for mixtures at a constant surfactant concentration of 100 mM and different TEA/Li ratios at a temperature of 30 °C. SANS curves were obtained either from the fluorinated micellar core or from the hydrogenated counterion atmosphere surrounding the micelles applying contrast matching. A transitional change in shape from spherical to prolate micelles was observed for TEA fractions greater than 30 mM. For TEA fractions greater than 55 mM, threadlike micelle structures are present. From the SANS data we are able to correlate the counterion binding of the two different species to the shape and size of the micellar structure and confirm the role that the counterion environment plays in macroscopic rheological properties.

10:00AM X8.00007 Fabrication of phospholipid vesicles from double emulsions in microfluidics, INSUN YOON, Mount Holyoke College, ANDERSON H. SHUM, DAEYON LEE, DAVID A. WEITZ, School of Engineering and Applied Sciences, Harvard University — Phospholipids self-assemble into lipid vesicles also known as liposomes. The formation of liposomes via conventional techniques such as electroformation has been studied extensively. However, the liposomes formed through electroformation are polydisperse and have low encapsulation efficiency. We present a new method to fabricate monodisperse phospholipid vesicles with high encapsulation efficiency from water-in-oil-in-water double emulsions. We generate phospholipid stabilized monodisperse double emulsions using a glass microcapillary device. This process allows efficient encapsulation within the inner aqueous drop. The middle oil phase is a volatile organic solvent in which phospholipids are dissolved. As the organic solvent evaporates, phospholipids self-organize into vesicles. This technique is versatile in the choice of phospholipids and we have generated vesicles from different types of phospholipids.
We find that although these dynamics are difficult to observe in traps, it is possible to observe them in optical lattices; particularly they can survive in $F=2$ optical lattices. These dynamics have unique dependence on quadratic Zeeman fields and potential depth in optical lattices. Quantum fluctuation-controlled spin dynamics are sensible to the variation of fluctuations and the potential induced by quantum fluctuations can be tuned by a biaxial spin nematic. Recently we also study coherent spin dynamics mainly driven by quantum fluctuations. Unlike the usual mean-field driven dynamics, hyperfine spin $F=2$ dynamics of hyperfine spin $F=2$ Cold Atoms.

Also at National Institute of Standards and Technology

Friday, March 14, 2008 8:00AM - 10:48AM – Session X9 DAMOP: Focus Session: Spinor Condensates and Dipolar Gases Morial Convention Center

10:12AM X8.00008 Concentration dependence of dynamics of a droplet microemulsion, MICHIHIRO NAGAO, Indiana University, HIDEKI SETO, Kyoto University, Japan — We will present a concentration dependence of dynamics of a spherical droplet microemulsion, consisting of aerosol-OT (AOT), as a surfactant, water, and decane. This mixture forms spherical microemulsion in a wide range of concentration. With keeping water to surfactant ratio constant, concentration of water plus surfactant was changed. The static structure of this system has been determined by small-angle neutron scattering (SANS) using the relative form factor method in the droplet concentration range from 5 to 75 % [1].

Dynamics of droplet microemulsions have been determined using neutron spin echo technique, which is suitable to measure dynamics of systems in nanometer and nanosecond scales. We measured dynamics of the system at 5, 30, and 60 % of droplet concentration. Using analogous data reduction procedure to SANS, contribution of shape fluctuations is decoupled from structure fluctuations. Concentration dependence of shape fluctuations and structure fluctuations will be discussed. [1] M. Nagao et al., Phys. Rev. E 75, 061401 (2007).

10:24AM X8.00009 Dielectrophoresis of Functional Phospholipid Vesicles, VICTORIA FROUDE, YINGXI ELAINE ZHU, University of Notre Dame — Recently, there has been an emerging interest in using AC-dielectrophoresis (DEP) to transport and assemble phospholipid vesicles (liposomes) and nanoparticles to form functional bio-assembly where the underlying charge polarization mechanism of colloids in AC fields strongly depends on nano-scaled surface charge. In this work, we study liposomes segregation and aggregation in the presence of nanocolloids and salts in which the biological functionality of liposomes is augmented by the physical functionality of inorganic coating and particles. Liposomes, synthesized by sonication with L,2-Dioleoyl-sn-Glycero-3-Phosphate (DOPA), are manipulated at varied AC-field frequencies across fabricated micro-electrodes in a quadrupole configuration on glass. We observe the co-assembly of liposome and opposite-charged nanocolloids by confocal microscopy and SEM, where the smaller nanocolloids are captured in between liposome junctions to form stabilized composite vesicles at several distinct frequencies. We observe a strong dependence of the liposome DEP mobility on the number of nanoparticles present in suspension and propose a new mechanism based on charge segregation and charged nanocolloid entainment in the double layer.

10:36AM X8.00010 High-throughput Microsphere Encapsulation in Emulsion Droplets by Electrospray, WUEN-SHIU CHEN, KENG-HUI LIN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Colloidal clusters generated through emulsion encapsulation and evaporation open up the possibilities for assembly of complex crystal structures. Encapsulation in monodisperse emulsion droplets facilitates higher yield of identical clusters as building blocks. We utilize electrospray in an oil-in-water co-flow fluidic device to generate uniform emulsion droplets in micron size and at the rate of ten thousand droplets per second. We investigate the effect of applied voltage, flow rate and the conductivity of liquid on the droplet formation. We further show that incorporation of microspheres into the inner oil fluid enables the encapsulation and formation of clusters.

8:00AM X9.00001 Amplification of quantum fluctuations across a quantum phase transition in a spinor BEC, SABRINA LESLIE, JENNIE GUZMAN, MUKUND VENGALATTORE, DAN STAMPER-KURN, Department of Physics, UC Berkeley — We study the amplification of quantum fluctuations in a $^{87}$Rb spinor BEC that is rapidly quenched from its paramagnetic phase to its ferromagnetic phase. By characterizing the onset of spontaneous ferromagnetism and the amplification properties of the spinor condensate, we probe the initial quantum fluctuations from which the resulting structures evolve. To characterize the spinor condensate as an amplifier, we temporally and spatially resolve the evolution of the vector magnetization profile as a function of the end point of the quench. In particular, we describe the formation of transversely magnetized domains and vortices as a function of the end point.

8:12AM X9.00002 Equilibrium phases of a dipolar spinor Bose gas, MUKUND VENGALATTORE, S. R. LESLIE, J. GUZMAN, C. SMALLWOOD, D. M. STAMPER-KURN, University of California, Berkeley — We investigate the effect of magnetic dipole interactions in determining the properties of $F = 1$ spinor Bose gases of $^{87}$Rb. Due to the competition between the local ferromagnetic interaction and the long-range, anisotropic dipole interaction, we observe the spontaneous formation of modulated spin domains that exhibit crystalline order. The formation of this modulated spin texture is accompanied by the creation of spin vortices in this dipolar superfluid. We observe this modulated phase both as an equilibrium phenomenon by cooling an incoherent thermal spinor gas, and as a result of a dynamical instability in a pure transversely magnetized spinor condensate. We clarify the crucial role played by dipolar interactions in the creation of the crystalline phase in the spinor condensate and study the finite temperature phase diagram of this dipolar quantum fluid.

8:24AM X9.00003 Dynamical instability of the XY spiral state of ferromagnetic condensates, ROBERT CHERNG, VLADIMIR GRITSEV, Harvard University, DAN STAMPER-KURN, University of California, Berkeley, EUGENE DEMLER, Harvard University — We calculate the spectrum of collective excitations of the XY spiral state prepared adiabatically or suddenly from a uniform ferromagnetic $F = 1$ condensate. For spiral wavevectors past a critical value, spin wave excitation energies become imaginary indicating a dynamical instability. We construct phase diagrams as functions of spiral wavevector and quadratic Zeeman energy.

8:36AM X9.00004 Spin Nematics and Quantum Fluctuation-Controlled Coherent Spin Dynamics of Hyperfine Spin $F=2$ Cold Atoms, JUN LIANG SONG, GORDON SEMENOFF, FEI ZHOU, The University of British Columbia — We show that quantum fluctuations lift the accidental continuous degeneracy that was found in the mean field analysis of spin nematic states of hyperfine spin $F=2$ $^{87}$Rb. Two distinct spin nematic states with higher symmetries are selected out depending on scattering lengths: a uniaxial spin nematic and a biaxial spin nematic. Recently we also study coherent spin dynamics mainly driven by quantum fluctuations. Unlike the usual mean-field driven dynamics, quantum fluctuation-controlled spin dynamics are sensible to the variation of fluctuations and the potential induced by quantum fluctuations can be tuned by four or five orders of magnitude in optical lattices. These dynamics have unique dependence on quadratic Zeeman fields and potential depth in optical lattices. We find that although these dynamics are difficult to observe in traps, it is possible to observe them in optical lattices; particularly they can survive in $F=2$ $^{87}$Rb condensates with a relatively short life time.

This work is supported by the office of the Dean of Science, University of British Columbia, NSERC(Canada), Canadian Institute for Advanced Research, and the Alfred P. Sloan foundation.
8:48AM X9.00005 Nematic order by disorder in spin-2 BECs. RYAN BARNETT, Caltech, ARI TURNER, EUGENE DEMLER, Harvard, ASHVIN VISHWANATH, Berkeley — The effect of quantum and thermal fluctuations on the phase diagram of spin-2 BECs is examined. They are found to play an important role in the nematic part of the phase diagram, where a mean-field treatment of two-body interactions is unable to lift the accidental degeneracy between nematic states. Quantum and thermal fluctuations resolve this degeneracy, selecting the uniaxial nematic state, for scattering lengths a₁ greater than a₂, and the square biaxial nematic state for a₂ less than a₁. Paradoxically, the fluctuation induced order is stronger at higher temperatures, for a range of temperatures below T_c. For the experimentally relevant cases of spin-2 ⁸⁷Rb and ⁴⁰K, we argue that such fluctuations could successfully compete against other effects like the quadratic Zeeman field, and stabilize the uniaxial phase for experimentally realistic conditions. A continuous transition of the Ising type from uniaxial to square biaxial order is predicted on raising the magnetic field. These systems present a promising experimental opportunity to realize the ‘order by disorder’ phenomenon.

9:00AM X9.00006 ABSTRACT WITHDRAWN —

9:12AM X9.00007 Ultracold dipolar gases — challenge for Experiments and Theory. MIKHAIL BARANOV, Universiteit van Amsterdam — Recent experimental progress in trapping and cooling of molecular gases boosts an interest to the interdisciplinary field of quantum gases with dominant dipole-dipole interactions. An unprecedented level of experimental control together with specific physical properties of the dipole-dipole interaction provides a unique possibility to find new physical phenomena and practical applications. In this talk, recent achievements in studies of ultracold dipolar gases, both fermionic and bosonic, are presented. We focus our attention on many-body properties of such systems and discuss how the characteristic features of the dipole-dipole interaction: long range and anisotropy, affect their collective behavior and result in novel macroscopic quantum phenomena.

9:48AM X9.00008 Spin-orbit interaction effects in cold atomic systems. TUDOR STANESCU, VICTOR GALITSKI, University of Maryland — We propose a scheme for the realization of spin-orbit interaction in cold atomic systems. We show that, in a system of trapped multi-level atoms moving in the presence of spatially modulated laser fields, the atom-laser interaction generates an emergent pseudo-spin-1/2 degree of freedom that couples to the momentum, leading to an effective spin-orbit interaction. The parameters of the spin-orbit coupling can be modified by controlling the laser fields. Atomic spin-orbit interacting systems open the possibility of studying new effects that are not usually considered, or not accessible in solid state systems. We consider explicitly the problem of strongly non-equilibrium spin dynamics by studying the evolution of an initially spin-polarized Fermi gas in a two-dimensional harmonic trap. We derive the non-equilibrium behavior of the polarization and show that it is characterized by periodic echoes with a frequency equal to the trapping frequency. We also consider a system of multi-level Bose atoms. In the presence of spin-orbit coupling, the single-particle band structure is generally anisotropic and contains two minima at finite momenta. At low temperatures, the bosons condense into these states, leading to a new type of Bose-Einstein condensate.

10:00AM X9.00009 Dipolar bosons in an array of one-dimensional tubes¹. JULIA S. MEYER, The Ohio State University, CORINNA KOLLATH, Centre de Physique Theorique, Ecole Polytechnique, THIERRY GIAMARCHI, University of Geneva, DPMC-MaNEP — Ultra-cold atomic and molecular gases offer a unique possibility to realize a range of novel interacting many-body systems. While in solid state systems electrons interact via the long-range Coulomb interactions, the interactions in cold gases are essentially local. However, the use of dipolar atoms or molecules allows one to surmount this limitation. We investigate bosonic atoms or molecules interacting via dipolar interactions in a planar array of one-dimensional tubes. In the situation where the dipoles are oriented perpendicular to the tubes by an external field, various quantum phases can be realized by varying the strength of the interactions and the orientation of the dipoles with respect to the plane of the array. We find a ‘sliding Luttinger liquid’ phase in which the tubes remain Luttinger liquids and two-dimensional charge density wave ordered phases with different kinds of order. In particular, a stripe phase in which the bosons in different tubes are aligned as well as a checkerboard phase occur.

¹ This work was supported in part by the U.S. DOE, Office of Science, under Contract No. DE-FG02-07ER46424 and by the Swiss NSF under MaNEP and Division II.

10:12AM X9.00010 Phase space deformation of dipolar Fermi gas². HAN PU, Rice University, TAKAHIKO MIYAKAWA, Tokyo University of Science, TAKAARI SOGO, Kyoto University, HONG LU, Rice University — We consider a system of quantum degenerate spin polarized fermions in a harmonic trap at zero temperature, interacting via dipole-dipole forces. Under the semi-classical framework, we introduce a variational Wigner distribution function to characterize the deformation and compression of the Fermi gas in phase space and use it to examine the stability of the system. We emphasize the important roles played by the Fock exchange term of the dipolar interaction which results in a non-spherical Fermi surface.

²This work is supported by NSF, the Keck Foundation and MEXT of Japan.

10:24AM X9.00011 ABSTRACT WITHDRAWN —

10:36AM X9.00012 Towards Microwave Trapping of Cold Polar Molecules¹. Y.-C. CHEN, C.-C. HSIEH, T.-S. KU, P. DWIVEDI, R. HO, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan — We describe our progress on production and trapping of cold SrF molecules. Specifically, we generate the SrF molecules by laser ablation of its solid precursor. We use helium buffer gas cooling as the first cooling stage to cool molecules down to a few Kelvin. To guide the generated cold molecules to ultrahigh vacuum region for further spectroscopic studies and trapping, we are also developing the electrostatic guiding of molecules. The experimental results will be presented. For a second-stage cooling in order to cool molecules down to ultracold regime, we plan to perform the sympathetic cooling of molecules with ultracold cesium atoms in a microwave trap. We have succeeded to build a microwave trap based on a high-power microwave Fabry-Perot resonator. We can couple 1.4 kW power into the cavity with a coupling efficiency more than 80% under locked conditions. The trap depth for the absolute ground state of SrF molecules is 300mK. The design and performance as well as future improvements will be discussed in details.

¹We acknowledge the support from National Science Council of Taiwan and Academia Sinica.

Friday, March 14, 2008 8:00AM - 11:00AM —
Session X10 DCMP: Superconducting Devices and Applications  Morial Convention Center RO8
8:00AM X10.00001 A tunable parametric amplifier based on a SQUID array resonator with nearly quantum-limited sensitivity, MANUEL CASTELLanos-BELTRAN, KONRAD LEHNERT, JILA, NIST and the University of Colorado, and the Department of Physics, University of Colorado, Boulder, Colorado 0309-0440, USA. — Recently, there has been an increasing number of compelling applications for quantum-limited amplifiers at microwave frequencies. These include the readout of superconducting qubits and ultrasensitive measurements of the motion of nanomechanical beams. Although quantum-limited microwave amplifiers have already been demonstrated, they have suffered from both limited bandwidth and dynamic range. We create a Josephson parametric amplifier from a transmission line resonator whose inner conductor is made from a series SQUID array. By changing the magnetic flux through the SQUID loops, we are able to adjust the circuit’s resonance frequency and, consequently, the center of the amplified band over an octave (4-8 GHz). This tunability circumvents some of the problems related to a limited bandwidth. We will discuss recent results that include demonstration of large gain (30 dB), nearly quantum-limited sensitivity and noise squeezing.

8:12AM X10.00002 Parametric amplification in a DC SQUID amplifier at 1.7 GHz, JOSE AUGMENTADO, LAFE SPIETZ, K.D. IRWIN, NIST — At NIST we have recently developed a DC SQUID-based microwave amplifier employing a resonant input circuit. In conventional operation this amplifier can be operated in a linear, phase-preserving mode. However, it can also be operated as a degenerate parametric amplifier with the SQUID functioning as a first stage amplifier. We will discuss the performance of this hybrid operation and the possibility of generating squeezed states in this system.

8:24AM X10.00003 Progress at NIST on DC SQUID Microwave Amplifiers, LAFE SPIETZ, K. D. IRWIN, J. AUGMENTADO, NIST — We report on the development at NIST of microwave amplifiers using DC SQUIDs. Our design approach is to use small SQUIDs which can be modeled as lumped element circuits, thus separating the design process for the SQUID from that of the microwave impedance transformers. We present our model of the impedance, gain and noise of such a SQUID and measurements of the characteristics of our amplifiers.

8:36AM X10.00004 Input Impedance of the Microstrip SQUID Amplifier, DARIN KINION, Lawrence Livermore National Laboratory, JOHN CLARKE, Physics Department, University of California Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We present measurements of the complex scattering parameters of microstrip SQUID amplifiers (MSA) cooled to 4.2 K. The input of the MSA is a microstrip transmission line in the shape of a square spiral coil surrounding the hole in the SQUID washer that serves as the ground plane. The input impedance is found by reversing the scattering parameter (S11) and is described well by a low-loss transmission line model. We map the low-loss transmission line model into an equivalent parallel RLC circuit in which a resistance R, inductance L, and capacitance C are calculated from the resonant frequency, characteristic impedance and attenuation factor. Using this equivalent RLC circuit, we model the MSA and input network with a lumped circuit model that accurately predicts the observed gain given by the forward scattering parameter (S21). We will summarize results for different coil geometries and terminations as well as SQUID bias conditions. A portion of this work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory in part under Contract W-7405-Eng-48 and in part under Contract DE-AC52-07NA27344 and by Lawrence Berkeley National Laboratory under Contract No. DE-AC02-05CH11231.

8:48AM X10.00005 In vivo T1 maps at fields from 0.001 to 150 mT with SQUID based MRI, M. HATRIDGE, S. BUSCH, T. WONG, M. MOESSLE, A. PINES, J. CLARKE, UC Berkeley/LBNL — High field magnetic resonance imaging (MRI) uses differences in the longitudinal relaxation times (T1) of protons to differentiate tissue types. Using phantoms and ex vivo human tissue, we have demonstrated that T1 contrast at low fields can be much greater than that at high fields, suggesting that one can, for example, distinguish tumors from healthy tissue without the use of contrast agents. Our MRI system polarizes protons at fields up to 150 mT using a water-cooled electromagnet. Subsequently, we ramp down the polarizing field and measure the proton nuclear magnetic resonance at typically 0.132 mT in the presence of three-dimensional field gradients using a SQUID coupled to an untuned, second-derivative gradiometer. Our system is capable of imaging the human arm in vivo with a resolution of 2x2x10 mm3. By switching the field to an intermediate field value for a variable time, we can obtain T1 maps at fields between 0.001 and 150 mT. We present in vivo T1 dispersion curves in the same range of magnetic fields for several types of tissue in the human arm. Work supported by USDOE.

9:00AM X10.00006 Fast, single-photon detection with a superconducting Nb nanowire, ANTHONY ANNUNZIATA, ANDREW MACK, JOEL CHUDOW, DANIEL SANTAVICCA, Yale University, AVIAD FRYDMAN, Bar Ilan University, MICHAEL ROOKS, IBM - Watson Research Center, LUIGI FRUNZIO, DANIEL PROBER, Yale University — We investigate the performance of a superconducting nanowire detector made from an ultra-thin, pure Nb film. Single photon counting performance is shown with good quantum efficiency at 470 nm. We report the reset time, jitter, and dark count rate for single photon detection. We compare these results to reports for NbN detectors. The Nb detector has a faster reset time for the same size active area, with similar quantum efficiency. These detectors have a variety of potential applications ranging from VLSI circuit diagnostics to quantum communication and single molecule spectroscopy. This work is supported by NSF – EPDT and IBM research.

9:12AM X10.00007 Local superfluid densities probed via current-induced superconducting phase gradients, ALEXEY BEZRYADIN, University of Illinois at Urbana-Champaign, DAVID HOPKINS, LAM research, DAVID PEKKER, Harvard University, TZU-CHIEH WEI, University of Waterloo, PAUL GOLDBART, University of Illinois at Urbana-Champaign — We have developed a superconducting phase gradiometer consisting of two parallel DNA-templated nanowires connecting two thin-film leads [1,2,3]. We have ramped the cross current flowing perpendicular to the nanowires, and observed oscillations in the lead-to-lead resistance due to cross-current-induced phase differences. By using this gradiometer we have measured the temperature- and magnetic-field dependence of the superfluid density, and observed an amplification of phase gradients caused by elastic vortex displacements. We examine our data in light of Miller-Bardeen theory of dirty superconductors and a microscale version of Campbell’s model of field penetration.


This work supported by DOE Grants No.DEFG02-07ER46453 and No. DEFG02-91ER45439 and by NSF DMR Grant No. 0134770.

9:24AM X10.00008 Entanglement of Two Josephson Vortex Quantum Bits in Resonant Cavity, ISAAC O’BRYANT, RAMESH P. DHUNGANÀ, JU H. KIM, University of North Dakota — We investigate the entanglement between two Josephson vortex qubits (JQV’s) in a resonant cavity. A JQV may be fabricated using two closely spaced microresistor sites in an insulator layer of a long Josephson junction. The phase dynamics of a Josephson vortex (or fluxon) may be described using the perturbed sine-Gordon equation. In a uniform electromagnetic field, it is found that the resonant cavity interacts with fluxons only when they are trapped on a microresistor. The effect of a resonant cavity on the two JQV’s may be represented as a deformation of the two-qubit potential function. We examine the effects of resonant cavity and magnetic induction on the potential for two non-interacting JQV’s. The deformation of the potential due to the resonant cavity yields a significant increase in the two-fluxon tunneling compared to the single-fluxon tunneling, indicating that entanglement between the two JQV’s is significantly increased. We compute the concurrence to estimate how the entanglement is affected by the magnetic induction effect and the coupling between the fluxons and the resonant cavity.
9:36AM X10.00009 Death of entanglement of two Josephson vortex qubit due to the dissipation effect, RAMESH DHUNGANA, ISAAC O'BRYANT, JU KIM, University of North Dakota — We investigate the effects of the dissipation on the two entangled Josephson vortex qubits (i.e. JVQ) using spin-boson model. It has been suggested that the decoherence time for a JVQ can be longer than the time for which it can be measured because it couples only weakly to the sources of decoherence. The entanglement of two JVQs due to the magnetic induction effect between two long Josephson junctions and their coupling to a single mode resonant cavity may be destroyed due to the same source of decoherence, which are present in the environment. We consider the decoherence effect on the JVQ system by using a dissipative thermal bath. We estimate its effect on entanglement, which can be measured in terms of concurrence, to show that the entanglement may die down quickly due to the decoherence once. We compare the entanglement survival of two JVQs in the dissipative environment with the decoherence time for a single JVQ qubit and discuss its effect on the two qubit operation.

9:48AM X10.00010 Probing Temperature Dependent Noise in Flux Qubits via Macroscopic Resonant Tunneling, A.J. BERKLEY, R. HARRIS, M.W. JOHNSON, J. JOHANSSON, P. BUNYK, S. GOVOROV, M.C. THOM, S. UCHAarkin, C.J.S. TRUINcK, M.H.S. AMIN, D-Wave Systems Inc. — 100-4401 still Creek Dr., Burnaby, BC V5C 6G9, Canada, S. HAN, Department of Physics and Astronomy, University of Kansas, Lawrence KS, USA, B. BUMBLE, A. FUNG, A. KAUL, A. KLEINsasser. Jet Propulsion Laboratory, California Institute of Technology, Pasadena CA, USA, D.V. AVERIN, Department of Physics and Astronomy, SUNY Stony Brook, Stony Brook NY, USA — Macroscopic resonant tunneling between the two lowest lying states of a bistable RF-SQUID is used to characterize flux noise in a potential qubit. Detailed measurements of incoherent decay rates as a function of flux bias revealed that the Gaussian shaped tunneling rate is not peaked at the resonance point, but is shifted to a flux bias at which the internal well is higher than the target well. This observation indicates that the dominant low frequency (1/f) flux noise in this device is quantum mechanical in nature. The r.m.s. amplitude of the noise, which is proportional to decoherence rate 1/T_2, was observed to be weakly dependent on temperature below 70 mK.

10:00AM X10.00011 Simulation of a YBCO Superconducting Quantum Interference Filter, STEPHEN M. WU, SHANE A. CYBART, JOHN CLARKE, R.C. DYNES, Physics Department, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — A Superconducting Quantum Interference Filter (SQUIF) consists of a serial or parallel combination of SQUIDS of varying area that at constant current bias produces a sharp voltage peak at zero magnetic field. We simulated a series array of 300 SQUIDS to calculate the voltage response versus applied magnetic field. We chose representative values of the junction critical current I_c and resistance R_N for YBCO Josephson junctions. We varied the areas to maximize the sharpness and height of the voltage peak. We used the results of the simulation to design a SQUIF that we fabricated and tested. The measured voltage response of the device was smaller than the predictions of the model. The agreement was significantly improved by including the effects of the geometric inductances of the SQUID loops and the Fraunhofer diffraction pattern of the individual junctions, both of which reduced the predicted amplitude of the SIF response. It is likely that the remaining discrepancies are due partly to random variations in I_c and R_N in the experimental device, which we shall include in future simulations, and partly to the effects of thermal noise. This work was supported by AFSOR.

10:12AM X10.00012 Measurements of a YBCO superconducting quantum interference filter with planar ion-damaged Josephson junctions, SHANE A. CYBART, S. WU, J. SIDDIOI, JOHN CLARKE, R.C. DYNES, Department of Physics, University of California Berkeley and Material Science Division, Lawrence Berkeley National Laboratory — We have fabricated a superconducting quantum interference filter (SQUIF) containing 300 SQUIDS connected in series. Loops in a YBCO film were patterned using photolithography and argon ion milling. The Josephson junctions were formed with ion bombardment through 30 nm wide slits that were patterned with electron beam lithography and reactive ion etching of a 25 nm germanium / 800 nm photoresist mask. The ion damage lowered the Tc of the 30 nm unmasked region resulting in SS's junctions, where supercondconductor S has a Tc of 85 K, and S' of 75 K. The IcRn product for individual junctions was determined to be 0.02 mV from current-voltage characteristics measured at 73K. Voltage versus magnetic field curves were measured for different static bias currents. They show a dip at zero field which increases with increasing bias up to a saturation value of 2 mV. The maximum transfer coefficient was 17 mV/mT. Noise properties and linearity measurements will be presented. This work was supported by AFOSR, and by DOE through the LBLN Molecular Foundry.

10:24AM X10.00013 Fabrication and evaluation of the superconducting d-dot device manufactured with the Y_{0.9}La_{0.1}Ba_{1.9}Cu_{3}O_{y} thin film by a DC Sputtering method, MASAHIDE NISHIYAMA, Osaka Pref. Univ. & JST-CREST, HIROAKI SATO, Osaka Pref. Univ., MASUO YAMAMOTO, Osaka Pref. Univ. & JST-CREST, SEIJI ADACHI, HIRONORI WAKANA, KEICHII TANABE, SRL-ISTEC, TAKAKAZU ISHIDA, Osaka Pref. Univ. & JST-CREST — The d-dot device is composed of a square shaped d-wave superconductor buried into a s-wave superconductor thin film. The internal phase difference at neighboring square side junction causes a half-quantum-flux at each corner of square of d-wave superconductor. We have developed the method for preparing the d-dot with YBCO thin film by PLD method previously. In the present work, we employed a DC sputtered Y_{0.9}La_{0.1}Ba_{1.9}Cu_{3}O_{y} thin film with ramp edge, which is a well-established standard process for fabricating high-T_{c} single flux quantum (SFQ) device of SRL-ISTEC. Evaluations of this d-dot device are performed by I-V and R-T measurements. The magnetic flux structure has been investigated by a scanning SQUID microscope.

10:36AM X10.00014 High frequency flux sampling SQUID microscope, CONSTANTINE VLHACOS, C.NAM, Department of Electrical and Computer Engineering, University of Maryland College Park and the Laboratory for Physical Sciences, JOHN MATTHEWS, Physics Department, University of North Carolina — We have fabricated a high frequency flux sampling SQUID microscope. This device is based on a high-T_{c} superconducting thin film Y_{0.9}La_{0.1}Ba_{1.9}Cu_{3}O_{y}, which is grown on a sapphire substrate. The SQUID is a single flux quantum device which is fabricated using a standard process for high-T_{c} thin film technology. The SQUID is a single flux quantum device which is fabricated using a standard process for high-T_{c} thin film technology. The SQUID is a single flux quantum device which is fabricated using a standard process for high-T_{c} thin film technology.

10:48AM X10.00015 Scanning Tunneling Microscopy Studies of AlN Tunnel Barriers, Y. LI, Cornell, J. READ, H. TSENG, R. BUHRMAN — Typical Josephson junctions (JJs) utilize alumina (AlO_{x}) tunnel barriers due primarily to the reliable thermal oxidation procedure that yield high quality Nb-Al-AlO_{x}-Nb JJs in the low and moderate (≤ 10^{2} A/cm²) critical current density (J_{c}) regime[1]. However, AlN provides the possibility of forming ultra-thin barriers with fewer defects, and hence lower sub-gap leakage currents, and thus could improve device performance in the high J_{c} regime [2-4]. We present results from an X-ray photoelectron spectroscopy (XPS) and scanning tunneling spectroscopy (STS) study of thin AlN layers on Nb formed by reactive radio frequency (rf) sputtering from an AlN target in a mixture of Ar and N gases. The XPS spectra indicates that O is generally incorporated into the nitride layer during growth in high and near-ultra-high vacuum, thus forming AlO_{x}N_{y}. The STS measurements reveal that these AlO_{x}N_{y} layers exhibit an increase in bandgap with increased N content in the process gas. Decreased band-tails and improved surface stability suggest the barrier deposition can be modified through moderate post-growth annealing. We will provide suggestions for optimization of rf sputtered AlO_{x}N_{y} layers for use in high J_{c} Nb and AlN based JJs. [1] Miller, APL 63, 1423 (1993) [2] Wang, APL 64, 2034 (1994) [3] Kleinsasser, IEEE TES 5, 2318 (1995) [4] Kaul, JMRs 20, 3047 (2005)
Symmetry properties and residual transport in superconducting PrOs$_4$Sb$_{12}$. TAYSEER ABU ALRUB, STEPHANIE CURNOE, Memorial University — We identify a three-component order parameter in the triplet channel as the most probable candidate for superconductivity in PrOs$_4$Sb$_{12}$. Two different superconducting phases have been observed in PrOs$_4$Sb$_{12}$; the lower temperature ‘B phase’ occupies the bulk of the phase diagram and breaks time reversal symmetry while the higher temperature ‘A phase’ found in a narrow region below H$_c$, and possibly does not exist at all. The gap function in the A phase is unitary and has two nodes in the [001] direction. In the B phase, the gap function is nonunitary and the lower branch has four cusp nodes in the $\{\pm x, \pm y, 0\}$ directions. The conductivity tensor, due to isotropic impurity scattering, has inequivalent diagonal components due to the off-axis nodal positions of the B phase.

This work was supported by NSERC of Canada.

Scanning SQUID imaging of Sr$_2$RuO$_4$ and PrOs$_4$Sb$_{12}$, CLIFFORD HICKS, JOHN KIRTLER, Department of Applied Physics, Stanford University, MARTIN HUBER, University of Colorado Denver, KATHRYN MOLER, Department of Applied Physics, Stanford University — We present scanning SQUID magnetometer data on the superconducting materials strontium ruthenate (Sr$_2$RuO$_4$) and praseodymium-osmium-antimonide (PrOs$_4$Sb$_{12}$), both of which are believed to have spin-triplet pairing and to generate spontaneous time-reversal-symmetry-breaking fields below their superconducting transition temperatures. Our images, taken with a SQUID with a resolution of 3μm and approximately 100μG, do not show evidence for spontaneous TRSB fields, in contrast with muon spin rotation data which indicates gauss-scale fields in both materials. The fields indicated by μSR data must therefore have a short length scale and/or a short time scale. Supposing that the TRSB fields are static with the magnitudes indicated by μSR data we place upper limits on their length scales in both Sr$_2$RuO$_4$ and PrOs$_4$Sb$_{12}$. We also place upper limits on the strength of any distributed fields that might exist at sample edges and order parameter domain walls.

This work was supported by the Department of Energy (DE-AC02-76SF00015).

Gauge-invariant electromagnetic response of a chiral $p_x+ip_y$ superconductor, ROMAN LUTCHYN, PAVEL NAGORNYKH, VICTOR YAKOVENKO, University of Maryland — We study electromagnetic properties of spin-triplet superconductors with chiral $p_x+ip_y$ symmetry of the pairing order parameter. As a result of spontaneously broken time-reversal symmetry, the electromagnetic response of $p_x+ip_y$ superconductor contains additional (anomalous) terms that are not present in conventional superconductors. Using effective action approach, we show that in $p_x+ip_y$ superconductors an external electric field may generate transverse Hall-like currents which depend explicitly on the chirality of the pairing order parameter. We also find an analog of the London equation in the anomalous electromagnetic response which implies complete screening of Cooper-pair intrinsic orbital momentum. The implications of our results to the experiments on Sr$_2$RuO$_4$ are discussed.

8:36 AM X11.00004 Stability of Half-Quantum Vortices in px-ipy Superconductors, SUK BUM CHUNG, University of Illinois at Urbana-Champaign, HENDRIK BLÜHM, EUN-AH KIM, Stanford University — We have analyzed the possibility of finding half-quantum magnetic vortices in a quasi-two-dimensional CHUNG, University of Illinois at Urbana-Champaign, HENDRIK BLUHM, EUN-AH KIM, Stanford University — We have analyzed the possibility of finding half-quantum magnetic vortices in a quasi-two-dimensional Sr$_2$RuO$_4$. Two different superconducting phases have been observed in PrOs$_4$Sb$_{12}$; the lower temperature ‘B phase’ occupies the bulk of the phase diagram and breaks time reversal symmetry while the higher temperature ‘A phase’ is found in a narrow region below H$_c$, and possibly does not exist at all. The gap function in the A phase is unitary and has two nodes in the [001] direction. In the B phase, the gap function is nonunitary and the lower branch has four cusp nodes in the $\{\pm x, \pm y, 0\}$ directions. The conductivity tensor, due to isotropic impurity scattering, has inequivalent diagonal components due to the off-axis nodal positions of the B phase.

This work was supported by Joint Quantum Institute Postdoctoral Fellowship(RL) and Graduate Assistantship (PN).

Angle-resolved Photoemission Study of Ca$_{1.8}$Sr$_{0.2}$RuO$_4$, MADHAB NEPANE, P. RICHARD, Z.-H. PAN, Y. XU, Department of Physics, Boston College, Chestnut Hill, MA 02467 USA, R. JIN, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 USA, X. DAI, Institute of Physics and National Laboratory for Condensed Matter Physics, Beijing, China, Z. WANG, H. DING, Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — We report angle-resolved photoemission spectroscopy results of the Fermi surface of Ca$_{1.8}$Sr$_{0.2}$RuO$_4$ which is at the boundary between a magnetic metal and an antiferromagnetic insulator in the phase diagram of the Ca-substituted strontium ruthenates. We did observe an orbital-selective Mott transition, which is, however, different with what has been predicted theoretically [1] for this material. Our ARPES results are consistent with both magnetic and transport properties observed in this material.


Superconducting pairing symmetries in the 3-K and bulk phases of Sr$_2$RuO$_4$, ZHENYI LONG, BENJAMIN CLouser, RONALD MEYER, SONGRUI ZHAO, KELLY MCCARTHY, YING LIU, Pennsylvania State University, HIROSHI YAGUCHI, YOSHITERU MAENO, Kyoto University, Japan, TIJIANG LIU, ZHIQIANG MAO, Tulane University — We report recent progress on our single-particle tunneling and phase-sensitive measurements on 3-K and bulk phases of Sr$_2$RuO$_4$. The latter refers to an electronic phase of Sr$_2$RuO$_4$ that features Ru microdomains embedded in a single crystal of Sr$_2$RuO$_4$. These Ru microdomains are of a mesoscopic size and varying shape. Therefore their pairing symmetries are not subject to the same set of constraints as those in the bulk. We have performed tunneling measurements on the 3-K phase to identify all possible pairing states in this unique superconducting system. The junctions used earlier were prepared by pressing In wire onto a cleaved ab face of a Ru-containing Sr$_2$RuO$_4$ single crystal containing multiple Ru microdomains. More recently we focused on tunnel junctions prepared on pre-selected single Ru microdomains. Possible existence of an intrinsic mixed pairing state in the interior of a Ru microdomain featuring simultaneous presence of both the $s$- and $p$-wave superconducting condensates. We will also discuss briefly our current effort in the phase-sensitive measurements on bulk Sr$_2$RuO$_4$, focusing on detecting possible $/k_F$ dependence of the order parameter and the existence of domains.
9:12AM X11.00007 Hall Conductivity in a Spin-Triplet Superconductor, WONKEE KIM, Texas Center for Superconductivity, F. MARSIGLIO, University of Alberta, C. S. TING, Texas Center for Superconductivity — We calculate the Hall conductivity for a spin-triplet superconductor, using a generalized pair ordering dependent on an arbitrary phase, \( \phi \). A promising candidate for such an order parameter is \( \text{Sr}_2\text{RuO}_4 \), whose superconducting order parameter symmetry is still subject to investigation. The value of this phase can be determined through Kerr rotation and DC Hall conductivity measurements. Our calculations impose significant constraints on \( \phi \).

9:24AM X11.00008 Upper Critical Field and SdH Quantum Oscillation Studies in Organic Superconductor \( \beta \)-(BEDT-TTF)\(_2\)SF\(_5\)CH\(_3\)CF\(_2\)SO\(_3\) \(-\text{(ET)}\)\(_2\)Cu[N(CN)\(_2\)]Br\(_2\) \(-\text{(BEDT-TTF)} \)\(_2\)SF\(_5\)CH\(_3\)CF\(_2\)SO\(_3\), KYUIL CHO\(^1\), BRAUNEN E. SMITH, WILLIAM A. CONIGLIO, LAUREL WINTER, CHARLES C. AGOSTA, Clark University, JOHN A. SCHLUETER, Argonne National Laboratory — Upper critical fields and SdH quantum oscillations in the organic superconductor \( \beta \)-(BEDT-TTF)\(_2\)SF\(_5\)CH\(_3\)CF\(_2\)SO\(_3\) have been studied by measuring the in-plane rf penetration depth with a tunnel diode oscillator technique. Previous measurements from other groups, with the applied field parallel to the conducting layers, were inconsistent. We report here that for the applied field parallel to the conducting layers the low temperature upper critical fields exceed the Pauli paramagnetic limit calculated by using a semi-empirical method. We will also discuss SdH quantum oscillation with the applied field perpendicular to the conducting layers, which has been found to have a frequency of 181 T and an effective mass of 1.84 m\(_e\). The effective mass is consistent with those of other groups, but the oscillation frequency smaller than theirs (~196 T).

\(^1\)We thank the DOE BES grant #ER46214 for support.

9:36AM X11.00009 Absolute penetration depth measurements in deuterated organic superconductor \( \kappa \)-(ET)\(_2\)Cu[N(CN)\(_2\)]Br\(_2\), TYSON OLHEISER, N. SALOVICH, R.W. GIANNETTA, University of Illinois at Champaign-Urbana, J. SCHLUETER, Chemistry and Materials Science Divisions, Argonne National Laboratory — Penetration depth measurements were performed on fully deuterated \( \kappa \)-(ET)\(_2\)Cu[N(CN)\(_2\)]Br, an organic superconductor. A novel aluminum plating technique was used to determine the absolute penetration depth \( \lambda(T) \). As the cooling rate is varied from 30 mK/min to 180 K/min we observe systematic changes in \( T_C \), superconducting fraction and \( \lambda(T) \). The data is analyzed using a model of superconducting domains embedded in an antiferromagnetic background.

\(^3\)Work at UIUC supported by NSF DMR 05-03882.

9:48AM X11.00010 Determination of the Pauli Paramagnetic Limit in Quasi 2D Superconductors\(^1\), BRAUNEN E. SMITH, KYUIL CHO, WILLIAM A. CONIGLIO, CHARLES C. AGOSTA, Clark University — We have calculated the Pauli paramagnetic limit (\( H_p \)) for different quasi 2D superconductors using a semi-empirical method. We then compared the calculated Pauli paramagnetic limits to penetration depth data obtained using a tunnel diode oscillator technique at low temperatures in a swept applied magnetic field. The organic superconductors examined are layered such that their behavior is dependent on their orientation to the applied magnetic field. In order to eliminate the effect of vortex dynamics, we examined data taken with the conducting layers oriented parallel to the applied magnetic field. For one of these materials, \( \kappa \)-(BEDT-TTF)\(_2\)Cu[N(CN)\(_2\)]Br, we find that eliminating vortex effects leaves us with one remaining feature in the data that may correspond to \( H_p \). We also find that the material \( \beta \)-(BEDT-TTF)\(_2\)SF\(_5\)CH\(_3\)CF\(_2\)SO\(_3\) exhibits a change in slope for temperature versus upper critical field when the upper critical field exceeds the calculated \( H_p \). In addition, many of the examined quasi 2D superconductors, including the above organic superconductors and CeColn\(_5\), exhibit upper critical fields that exceed their calculated \( H_p \), suggesting some type of non-conventional superconductivity.

\(^1\)We thank the DOE BES grant #ER46214 for support.

10:00AM X11.00011 Second harmonic magnetic field oscillations in LCSCO in magnetic fields, ALBERT MIGLIO, Los Alamos National Lab, JON BETTS, YOKO SUZUKI, LANL, IZABELA STROE, NHMFL TEAM — We describe a second harmonic technique to probe the thermal conductivity of LCSCO with superconductivity suppressed by high magnetic fields. The technique is suitable for the high noise environment of pulsed magnets. By subtracting the thermal conductivity in field and at zero field, we obtain information about the temperature dependence of the order parameter. Work performed under the auspices of the National High Magnetic Field Laboratory.

10:12AM X11.00012 Disorder induced weak and strong localization and their influence on superconductivity in underdoped Bi\(_2+\)xSr\(_2-x\)CuO\(_6\). HUIQIAN LUO, PENG CHENG, HAI-HU WEN, National Laboratory for Superconductivity, Institute of Physics, CAS — in-plane resistivity and magnetoresistance(MR) measurements were carried out on high-quality underdoped Bi\(_2+\)xSr\(_2-x\)CuO\(_6\), \( 0.1 \leq x \leq 0.4 \) single crystals. The results show that the superconductivity and the normal state MR behaviors strongly rely on the doping level of samples. In the slightly doping level of Bi, a metallic normal state and a finite superconducting transition temperature are observed, and there is always a positive MR in the normal state which is explained by the fluctuating superconductivity mixed with the transport of quasiparticles. With further doping, the low temperature resistivity shows an up turn together with a negative MR. Detailed analysis on the negative MR in this region may suggest that weak localization effect is dominant. As the superconductivity is depressed by more doping and thus more disorders, the delocalization gets much harder and the spin-order contribution may be involved in MR. Moreover, in the heavily underdoped doping, the superconductivity is suppressed completely and resistivity evolves into a strong localization behavior with a Coulomb gap opening at the Fermi energy. After summarizing the doping dependence of MR, we construct a new phase diagram to illustrate how does the disorder give the influence both on the superconductivity and magnetoresistance.

10:24AM X11.00013 Unusual diamagnetic response in p-wave superconductors \( \text{Sr}_2\text{RuO}_4 \), LU LI, JOSEPH CHECKELSKY, W. F. BRINKMAN, Department of Physics, Princeton University, M. KRIENER, Y. MAENO, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, NAI PHUAN ONG, Department of Physics, Princeton University — The magnetization \( M \) of the p-wave superconductor \( \text{Sr}_2\text{RuO}_4 \) has not been measured previously in the geometry with magnetic field \( H || c \) because of the small upper critical field \( (H_{c2} \approx 660 \text{ Oe}) \) and low \( T_c \) \((1.4 \text{ K})\). We have used high-resolution torque magnetometry to study in detail the magnetization curves in this geometry. We find that, in the superconducting state, the \( M-H \) curves display highly unusual hysteretic behavior. In the critical state, whenever \( H \) crosses zero, we observe a break in the slope \( \partial M/\partial H \). In a broad field interval \([ -H_c, H_0 ] \) bracketing zero field, \( M \) is reversible (to our resolution) under reversal of sweep direction. This anomalous behavior is not encountered in conventional type-II superconductors, where the critical-state behavior is always non-reversible. A possible interpretation of these unusual features is the existence of reversible edge currents. We also discuss the magnetization curves with \( H \parallel ab \), where \( M \) jumps sharply at \( H = H_{c2} \). Research supported by NSF grant DMR 0213706.
10:36AM X11.00014 Emergence of dissipative structures in current-carrying stabilized superconducting wires. GEORGE LEVIN, PAUL BARNES, Air Force Research Laboratory, JOSE RODRIGUEZ, Department of Physics and Astronomy, California State University, Los Angeles, JOHN BULMER, Air Force Research Laboratory, JAKE CONNORS, Ohio State University — We discuss the emergence of a dissipative structure in current-carrying superconducting wire. This is a phenomenon similar to the emergence of thermal convection cells, oscillatory chemical reactions, etc. In response to the initial localized temperature perturbation that leads to current exchange between the superconductor and the stabilizer the temperature and critical current density of the wire acquire spontaneous spatial modulation that forces the transport current to crosscross the interface between the superconducting film and metal stabilizer. This generates additional heat that makes such a structure self-sustainable. The central role in this phenomenon is played by the interfacial resistance between the stabilizer and superconducting film. The spatial scale of the modulation is of the order of the thermal diffusion length. This resistance also determines the speed of propagation of the conventional normal zone. We will present the results of numerical and analytical analysis of a model which describes current sharing between the superconducting and normal metal layers - a configuration typical of the state of the art YBCO-coated conductors.

10:48AM X11.00015 Thermoelectric effects and band-dependent scattering of normal-state quasiparticles in spin-triplet superconductor Sr$_2$RuO$_4$. ZHUAN XU, XIANGFAN GU, Zhejiang University, China, TIJIAN LIU, DAVID FOBES, ZHIQIANG MAO, Tulane University, YING LIU, Pennsylvania State University — We present the first measurement on Nernst effects in the normal state of odd-parity, spin-triplet superconductor Sr$_2$RuO$_4$. Below 100 K, the negative Nernst signal was found to be large and nonlinear as a function of magnetic field with its absolute value increasing rapidly as the temperature was lowered. After reaching a maximum around $T^* = 20 - 25$ K, however, the Nernst signal drops linearly with the decreasing temperature. No corresponding feature was found around this temperature in the specific heat. We argue that the large value of the Nernst signal is related to the presence of multibands and the nonlinearity to band-dependent magnetic fluctuation in Sr$_2$RuO$_4$. Furthermore, the quasiparticle scattering from the magnetic fluctuation is suppressed below $T^*$ due to the emergence of coherence among quasiparticles in the $\gamma$-band, an active band for superconductivity in Sr$_2$RuO$_4$. Results on temperature dependence of the thermopower, which was seen to exhibit a sharp kink around $T^*$, provided further support to this picture of band-dependent normal-state properties. Our thermoelectric measurements appear to suggest that the suppression of the magnetic fluctuation makes it possible for the spin-triplet superconductivity to emerge in Sr$_2$RuO$_4$. 

Friday, March 14, 2008 8:00AM - 10:36AM — Session X12 DCMP: Charge Density Wave and Charge Order Morial Convention Center 203

8:00AM X12.00001 Fermi Surface Evolution Across Multiple CDW Transitions in RTe$_3$. R.G. MOORE, Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, Menlo Park, CA 94025, V. BROUET, Laboratoire de Physique des Solides, Universite Paris-Sud, Bat 510, UMR 8505, 91405 Orsay, France. J. LAVEROCK, S. DUGDALE, H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom, R. HE, N. RUI, I.R. FISHER, Z.-X. SHEN, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, CA 94305 — The Fermi surface (FS) evolution across multiple charge density wave (CDW) transitions is investigated using angle-resolved photoemission spectroscopy. Low temperature measurements reveal two incommensurate CDW gaps created by perpendicular FS nesting vectors. A larger gap (≈250 meV) arising from a CDW with q$_{CDW} \sim 0.7c*$ is in good agreement with the expected trend determined from light rare earth members of the bi-layer family of rare earth trilivate compounds (RTe$_3$). A second, smaller gap (≈50 meV) is due to a second CDW with q$_{CDW} \sim 0.7a*$ never before seen in other RTe$_3$ compounds. The temperature dependence of the FS and the two CDW gaps is characterized.

1Work supported by DOE Office of Science, Division of Materials Science, with contract DE-FG03-01ER45929-A001 and NSF grant DMR-0604701.

8:12AM X12.00002 Momentum and time dependent electronic dynamics in the CDW compound TbTe$_3$. FELIX SCHMITT, Department of Applied Physics, Stanford University, Stanford, CA 94305, PATRIC KIRCHMANN, LAURENZ RETTIG, MARCEL KRENZ, Department of Physics, Freie Universitaet Berlin, Germany, NANCY RU, JUN-HAW CHU, Department of Applied Physics, Stanford University, Stanford, CA 94305, ROB MOORE, Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305, UWE BOVENSIEPEN, MARTIN WOLF, Department of Physics, Freie Universitaet Berlin, Germany, IAN FISHER, Department of Applied Physics, Stanford University, Stanford, CA 94305, ZHI-XUN SHEN, Department of Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305 — The rare earth tritellurides RTe$_3$ are charge-density-wave (CDW) systems in which the coupling strength can be tuned by substituting different rare earths. By using ultrashort IR pump and UV probe laser pulses, we have performed time resolved angular resolved electron photoemission spectroscopy (trARPES) on TbTe$_3$ and have observed the time-resolved closing of the CDW gap in the electronic band structure. To our knowledge, this is the first time-resolved study showing momentum dependent charge dynamics. We will also talk about other results on RTe$_3$ compounds.


8:36AM X12.00004 Quantum and classical mode softening near the charge-density-wave/superconductor transition of Cu$_3$TiSe$_2$: Raman spectroscopic studies. MINJUNG KIM, HARINI BARATH, S.L. COOPER, P. ABBAMONTE, E. FRADKIN, Dept. of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at U, E. MOROSAN, R.J. CAVA, Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — We report temperature- and x-dependent Raman studies of the charge density wave (CDW) amplitude modes in Cu$_3$TiSe$_2$, which allow us to study the temperature- and x-dependence of the soft mode in this system. Among the key results: we find that the A$_{2g}$ amplitude mode exhibits identical power law scaling with the reduced temperature, p(T/TCDW), and the reduced Cu content, p=x/\kappa, i.e., \omega_0 \sim (1-p)^{0.15}, suggesting that mode softening is independent of the control parameter used to approach the CDW transition; we provide evidence that x-dependent mode softening originates from the expansion of the lattice, which leads to a x-dependent reduction of the electron-phonon coupling constant; and we infer from our x-dependent mode softening results the presence of a quantum critical point, x_c(T=0)=0.07, within the superconducting phase of Cu$_3$TiSe$_2$.

3Work supported by the U.S. Department of Energy, Division of Materials Sciences, under Award Nos. DE-FG02-07ER46453 and DE-FG02-98-ER45706.
8:48AM X12.00005 Insulating charge density wave for a half-filled SU(N) Hubbard model with an attractive on-site interaction in one dimension. JIZE ZHAO, KAZUO UEDA, XIAOQUN WANG, The Institute for Solid State Physics, University of Tokyo — We study a one-dimensional SU(N) Hubbard model with an attractive on-site interaction and $N > 2$ at half-filling on the bipartite lattice using density-matrix renormalization-group method and a perturbation theory. We find that the ground state of the SU(N) Hubbard model is a charge density wave state with two-fold degeneracy. All the excitations are found to be gapful, resulting in an insulating ground state, in contrast to that in the SU(2) case. Moreover, the charge gap is equal to the Cooperon gap, which behaves as $-2N U^2/(N - 1)U$ in the strong coupling regime. However, the spin gap $\Delta_s$ and the quasiparticle gap $\Delta_1$ grow as well open exponentially in the weak coupling region, while in the strong coupling region, they linearly depend on $U$ such that $\Delta_s \sim -U(N - 1)$ and $\Delta_1 \sim -U(N - 1)/2$.

9:00AM X12.00006 Spin-soliton excitations from the Bond-Charge-Density Wave spin-Peierls state in the $1/2$-filled band. R.T. CLAY, R.P. HARDIKAR, Mississippi State University, S. MAZUMDAR, University of Arizona — The spin-Peierls (SP) transition is commonly discussed in the context of the $1/2$-filled band where the SP state is bond-dimerized. Spin excitations from the SP state generate spin solitons in pairs with opposite-phased bond alternation in between the solitons. As thermal excitations generate additional solitons, oppositely-phased regions overlap and ultimately give way to the uniform phase. Throughout the process, the charges on the sites remain uniform. This simple description has to break down in $1/2$-filled band systems where the SP state is a Bond-Charge-Density Wave (BCDW) state with coexisting bond and charge-tetramerization. At $1/2$-filled spin excitations are necessarily accompanied by changes in site charges. We prove the highly interesting result that site charges here can change locally in two different ways, leading to two different kinds of spin solitons. Which kind of soliton dominates is parameter-dependent. The two kinds of solitons promote two different high temperature states, which are either bond-dimerized or charge-dimerized. We discuss experimental consequences of our work.

1Supported by the Department of Energy grant DE-FG02-06ER46315.

9:12AM X12.00007 Measurements of the effect of charge density wave fluctuations on the $^{87}$Rb spin echo decay rate in Rb$_{0.30}$MoO$_3$. W.G. CLARK, GUOQING WU, S.E. BROWN, UCLA — Measurements and interpretation of the spin echo decay rate ($1/T_2$) for the $^{87}$Rb quadrupolar split satellite lines in the charge density wave (CDW) system Rb$_{0.30}$MoO$_3$ (blue bronze) are reported over the temperature ($T$) range 80 K to 250 K at several alignments of the magnetic field ($B = 9.00$ T). In contrast to the central transition, where the contribution of CDW fluctuations to $1/T_2$ is very small, they provide a large contribution to $1/T_2$ for the satellite lines below the CDW transition at $T_{CDW} \approx 180$ K. This sensitivity to CDW fluctuations shows that $1/T_2$ of the satellite lines should be a much more sensitive probe of both electric field driven and thermal motions of the CDW than the effects of density wave motion on the central transition, which has been used for prior work on this topic. A major goal of our future work is to exploit this property to obtain detailed measurements of electric field driven and thermal motion of the CDW in this material over a wide temperature range. This work has been supported by NSF Grants DMR-0334869 (WGC) and 0520552 (SEB).

9:24AM X12.00008 Electro-Optic Search for Critical Divergence of the Charge-Density-Wave Diffusion Constant at the Onset of Depinning in Blue Bronze. J.W. BRILL, L. LADINO, E.G. BITTLE, M. UDDIN, University of Kentucky — We have used electro-reflectance measurements to study charge-density-wave (CDW) polarization dynamics at voltages near the CDW depinning onset ($V_{on}$) in the quasi-one-dimensional conductor blue bronze. For low voltages, where the phase-slip rate is low, it is expected that the polarization relaxation time should be inversely proportional to the CDW diffusion constant, which is expected to diverge at $V_{on}$. At $T = 78$ K, we observe saturation of the relaxation time at low voltages, suggesting that we are in this low phase-slip, “elastic” limit and allowing us to estimate the non-critical value of the CDW diffusion constant $D(\infty) \sim 0.02$cm$^2$/s, consistent with the measured phonon velocity. At other temperatures, the relaxation time increases with decreasing voltage even at the lowest voltages we measure, indicating we are still dominated by phase-slip. In no case, however, do we observe the expected “critical speeding up”, setting an upper limit on the critical region of $V_1/V_{on} < 0.06$.

1Research supported by NSF grant DMR-0400938.

9:36AM X12.00009 Position and Current Dependence of Charge-Density-Wave Polarization Dynamics. L. LADINO, J.W. BRILL, University of Kentucky — We have studied the frequency and position dependence of charge-density-wave (CDW) polarization by simulating the response to square-waves of variable amplitude and frequency using parameters appropriate for niobium triselenide at $T = 90$ K, in its upper CDW state. For these simulations, we have numerically solved the phase-slip augmented diffusion model introduced by Adelman et al (Phys. Rev. B 54, 1833 (1996)) for time domain studies. At each position in the sample, the frequency dependence was fit to a modified harmonic oscillator expression and the position and current dependence of the fitting parameters determined. In particular, both the delay time ($1/\text{resonant frequency}$) and relaxation time decrease with increasing current (and phase-slip rate) and increase with distance from the contact, with the delay time vanishing adjacent to the contact, as experimentally observed with electro-optic measurements in blue bronze. No decay of the polarization at long times is observed however, in contrast to electro-optic results.

1Research supported by NSF grant DMR-0400938.

9:48AM X12.00010 Thermolectric studies of charge density wave dynamics. ROSS MCDONALD, NHMFL-Los Alamos, NEIL HARRISON, JOHN SINGLETON, NHMFL-LANL, TEAM CDW COLLABORATION — The conventional pyroelectric effect is intimately connected to the symmetry, or rather lack of center of symmetry, of the material. Although the experiments we discuss involve studies of low symmetry materials, the pyroelectric currents observed are of an entirely new origin. Systems with broken-translational-symmetry phases that incorporate orbital quantization can exhibit significant departures from thermodynamic equilibrium due to a change in magnetic induction. For charge density wave systems, this metastable state consists of a balance between the density-wave pinning force and the Lorentz force on the extended currents due to the drift of cyclotron orbits. In this way the density wave pinning potential plays a similar role to the edge potential in a two-dimensional electron gas, leading to a large Hall angle and quantization of the Hall resistance. A thermal perturbation that reduces the pinning potential returns the system towards thermal equilibrium, via a phason avalanche orthogonal to the sample surface. The observation of this new form of pyroelectric effect in the high magnetic field phase ($B > 30$ T) of the organic charge transfer salt $\alpha$-(BEDT-TTF)$_2$KHg(SCN)$_4$, thus provides a measure of the phason thermopower.
10:00AM X12.00011 Super-Crystalline CDW Phase in Organic Conductor (Per)$_2$Pt(mnt)$_2$\(^{1,2}\), SI WU, ANDREI LEBED, Dept. of Physics, Univ. of Arizona — We suggest a model \([1,2]\), where phase transitions between the Peierls and Super-Crystalline [or soliton wall superlattice (SWS)] charge-density-wave (CDW) phases occur in a magnetic field. The model accounts for peculiarities of an electron spectrum in a quasi-one-dimensional (Q1D) conductor (Per)$_2$Pt (mnt)$_2$. In particular, we show that the Pauli spin-splitting effects improve the nesting properties of a realistic Q1D electron spectrum, and, therefore, a high resistance Peierls CDW phase is stabilized in high magnetic fields. In low and very high magnetic fields, a periodic SWS (or Super-Crystalline) phase is found to be a ground state. We discuss \([3]\) possible experimental investigations of the theoretically predicted phase transitions in (Per)$_2$Pt(mnt)$_2$ to discover a unique SWS phase.

\[1\] Y.-J. Kao, L. Wang, and A. W. Sandvik (unpublished)


This work is supported by the Department of Energy grant DE-FG02-06ER46315.

10:12AM X12.00012 Temperature dependence of charge-ordering in (TMTCF)$_2$X, C = S, Se\(^{1}\), SUMIT MAZUMDAR, University of Arizona, RAHUL HARDIKAR, R. TORSTEN CLAY, Mississippi State University — Quasi one-dimensional 1/4-filled band charge transfer solids (CTS) undergo two distinct phase transitions as temperature decreases. At high temperature (\(\approx 100K\)) these materials undergo a 4K\(_X\) (period-two) charge or bond ordering transition. At low temperature, these CTS undergo a magnetic transition to either a spin-Peierls (SP) or anti-ferromagnetic (AFM) ground state, both of which coexist with charge-order (CO). Understanding the relationship between the high and low temperature CO states is a key problem here. We show that (i) the critical nearest neighbor Coulomb interaction V that drives the high temperature Wigner crystal CO is spin-dependent; (ii) as a consequence, for intermediate values of V, there occurs a transition from the Wigner crystal CO to a Bond-Charge-Density wave (BCDW) can occur as temperature decreases. This transition is consistent with recent NMR observations of a charge redistribution occurring simultaneously with the SP state. Our theory is able to explain the competition between the Wigner crystal and SP phases, as well as the occurrence of two difference AFM phases.

\[1\] This work is supported by the National Science Foundation.

10:24AM X12.00013 Infrared investigation of the charge ordering pattern in the organic spin ladder candidate (DTTTF)$_2$Cu(mnt)$_2$\(^{1}\), J.L. MUSFELDT, S. BROWN, University of Tennesse, S. MAZUMDAR, University of Arizona, R.T. CLAY, Mississippi State University, M. MAS-TORRENTE, C. ROVIRA, Institut de Ciencia de Materials de Barcelona, J.C. DIAS, R.T. HENRIQUES, M. ALMEIDA, Universidade de Lisboa — We measured the variable temperature infrared response of the spin ladder candidate (DTTTF)$_2$Cu(mnt)$_2$ in order to distinguish between two competing ladder models, rectangular versus zigzag, proposed for this family of materials. The distortion along the stack direction below 235 K is consistent with a doubling along \(b\) through the metal-insulator transition. While this would agree with either of the ladder models, the concomitant transverse distortion rules out the rectangular ladder model and supports the zigzag scenario. A mode analysis provides the microscopic basis for this distortion and an estimate for the degree of charge ordering. Intramolecular distortions within the DTTTF building block molecule also give rise to on-site charge asymmetry.

\[1\] This work is supported by the National Science Foundation.

Friday, March 14, 2008 8:00AM - 10:00AM — Session X13 DCOMP: Quantum Monte Carlo Methods and Strongly Correlated Systems

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8:00AM X13.00001 Variational approach for 1D antiferromagnetic Heisenberg chain with matrix-product states, YING-JER KAO, National Taiwan University, LING WANG, ANDERS SANDVIK, Boston University — In order to explore the practical applicability of variational Monte Carlo simulations based on matrix-product states (MPS) \([1]\), we present two implementations for the one-dimensional antiferromagnetic Heisenberg model with periodic boundary conditions \([2]\). We compare the convergence properties of two different schemes, which use either two sets of matrices corresponding to the two sublattices, or a 2-spin block representation. It is found that the use of symmetries considerably speeds up the convergence with the matrix size \(D\). We also present an efficient “cooling” schedule for the stochastic method used to optimize the matrices, which significantly reduces the computational effort. Finally, we will discuss application of the scheme to \(n\)-leg ladders with periodic boundary condition.


\[2\] Y.-J. Kao, L. Wang, and A. W. Sandvik (unpublished)

8:12AM X13.00002 Excited states from variational Monte Carlo simulations with matrix-product states\(^{1}\), LING WANG, Boston University, YING-JER KAO, National Taiwan University, ANDERS SANDVIK, Boston University — We report a further development \([1]\) of a recently proposed variational Monte Carlo method for matrix-product states (MPS) \([2]\). Using the frustrated \(J_1 - J_2\) Heisenberg chain as a test case, we show how the matrices can be optimized not just for the ground state, but also, simultaneously, for the lowest states in several different lattice and spin symmetry sectors. This is useful in, e.g., studies of quantum phase transitions associated with crossings of excited-state energies.

\[1\] Y.-J. Kao, L. Wang, and A. W. Sandvik (unpublished)


Supported by NSF Grant No. DMR-0513930.

8:24AM X13.00003 Scale-renormalized matrix-product states for correlated quantum systems\(^{1}\), ANDERS SANDVIK, Boston University — A generalization of matrix product states (MPS) is introduced which is suitable for describing interacting quantum systems in two and three dimensions. These \(\text{scale-renormalized matrix-product states (SR-MPS)}\) are based on a course-graining of the lattice in which the blocks at each level are associated with matrix products that are further transformed (scale renormalized) with other matrices before they are assembled to form blocks at the next level. Using variational Monte Carlo simulations of the two-dimensional transverse-field Ising model as a test, it is shown that the SR-MPS converge much more rapidly with the matrix size than a standard MPS. It is also shown that the use of lattice-symmetries speeds up the convergence very significantly.

Supported by NSF Grant No. DMR-0513930.
Cancer Treatment frequencies.

The phonon spectral function is given in both the metallic Luttinger liquid and the insulating charge density wave phase, for a wide range of phonon properties of the systems via momentum dependent phonon spectral functions and electron Greens functions. In case of the standard Holstein model, we present as well as Holstein type models, with momentum dependent couplings (e.g. breathing phonons) and arbitrary phonon dispersions. We access the dynamical EVERTZ, PETER PIPPAN, Techn. Univ. Graz — Using a QMC method based on exact phonon integration in Fourier space and on loop updates in particle state. For higher representation, we have not observed any VBS state, although the disappearance of the Neel order parameter has been detected as we increase N. from the Neel state to the VBS state around N=5 for the fundamental representation, we also find that there is an apparent U(1) symmetry in the VBS split-spin representation is used for high-dimensional representations. While we have confirmed our previous result[3] that the ground state switches University of Tokyo — The SU(N) generalization of the Heisenberg model is studied with a new loop algorithms with non-binary loop variables.[1] The[3] K. Harada, N. Kawashima and M. Troyer, Phys. Rev. Lett. 90...[24AM X13.00008 Spin waves and local magnetizations on the Penrose tiling . ATTILA SZALLAS, ANURADHA JAGANNATHAN, Laboratoire de Physique des Solides, CNRS-UMR 8502, Universite Paris-Sud, 91405 Orsay, France — The Penrose tiling is a perfectly ordered two dimensional structure with fivefold symmetry and scale invariance under site decimation. Quantum spin models on such a system can be expected to differ significantly from more conventional structures as a result of its special symmetries. We consider a Heisenberg antiferromagnet on the Penrose tiling, a quasiperiodic system having an inhomogeneous Neel-ordered ground state. Spin wave energies and wavefunctions are studied in the linear spin wave approximation. A linear dispersion law is found at low energies, as in other bipartite antiferromagnets, with an effective spin wave velocity lower than in the square lattice. Spatial properties of eigenmodes are characterized in several different ways. At low energies, eigenstates are relatively extended, and show multifractal scaling. At higher energies, states are more localized, and, depending on the energy, confined to sites of a specified coordination number. The ground state energy of this antiferromagnet, and local staggered magnetizations are calculated. Perpendicular space projections are shown, showing the underlying simplicity of this “complex” ground state. A simple analytical model, the two-tier Heisenberg star, is presented to explain the staggered magnetization distribution in this antiferromagnetic system.

8:36AM X13.00004 DMRG applied to quantum impurity models . ANDREAS WEICHSELBAUM, JAN VON DELFT, Ludwig Maximilian University — Quantum impurity models are analyzed routinely and reliably at very low energies using the Numerical Renormalization Group (NRG). Its great benefit of energy scale separation, however, comes at the cost of limited resolution at finite energy. By realizing that the NRG shares the same algebraic structure as the density matrix renormalization group (DMRG) given in terms of matrix product states, several strict NRG constraints such as its rigid discretization scheme in energy space can be relaxed due to the variational principle of DMRG. Our recent work in that respect will be discussed. 8:48AM X13.00005 Ameliorating the sign problem for frustrated magnets using plaquette grouping , KEVIN BEACH, University of Alberta — Frustrated quantum magnets are not amenable to simulation using conventional quantum Monte Carlo because of the infamous sign problem. In the overcomplete basis of singlet product states, updates have a many-to-one property that allows for grouping of updates around plaquettes in such a way that the negative sampling weights are almost entirely eliminated. Results for the J1-J2 quantum Heisenberg model on the square lattice are discussed.

9:00AM X13.00006 Bold Diagrammatic Monte Carlo: Generic Technique for Polaron Problems (and More?) , BORIS SVISTUNOV, NIKOLOY PROKOF’EV, University of Massachusetts, Amherst — We introduce a Monte Carlo scheme for sampling bold-line diagrammatic series specifying an unknown function in terms of itself. The range of convergence of this bold(-line) diagrammatic Monte Carlo (BMC) is significantly broader than that of a simple iterative scheme for solving integral equations. With BMC technique, a moderate “sign problem” turns out to be an advantage in terms of the convergence of the process. As an illustrative application, we solve the problem of fermipolaron (one spin-down particle interacting with the spin-up fermionic sea). The problem solved is prototypical for all polaron problems, and, probably, for many-particle systems as well.

9:12AM X13.00007 Interfacing Determinant Quantum Monte Carlo and Density Functional Theory1, NIKOLAI ZARKEVICH, University of California, Davis, CA 95616, ZHAOJUN BAI, Computer Science Department, University of California, Davis, CA 95616, SERGEY SAVRASOV, RICHARD SCALETTER, Physics Department, University of California, Davis, CA 95616, MARK JARRELL, Physics Department, University of Cincinnati, OH 45221 — Over the last decade many body theory and electronic structure calculations have come together within the “LDA+DMFT” approach in which dynamical mean field theory (DMFT) provides a frequency dependent self-energy \( \Sigma(\omega) \) for electronic structure calculation within the local density approximation (LDA). Here we describe initial results with a new approach which uses the determinant Quantum Monte Carlo method to supply the self energy. This technique has the advantage of providing a momentum dependent \( \Sigma(k,\omega) \). However, the fermion sign problem can limit the ability to access the ground state value of the self energy. We present tests of the approach on a model of cuprate superconductors.

9:24AM X13.00008 Spin waves and local magnetizations on the Penrose tiling . ATTILA SZALLAS, ANURADHA JAGANNATHAN, Laboratoire de Physique des Solides, CNRS-UMR 8502, Universite Paris-Sud, 91405 Orsay, France — The Penrose tiling is a perfectly ordered two dimensional structure with fivefold symmetry and scale invariance under site decimation. Quantum spin models on such a system can be expected to differ significantly from more conventional structures as a result of its special symmetries. We consider a Heisenberg antiferromagnet on the Penrose tiling, a quasiperiodic system having an inhomogeneous Neel-ordered ground state. Spin wave energies and wavefunctions are studied in the linear spin wave approximation. A linear dispersion law is found at low energies, as in other bipartite antiferromagnets, with an effective spin wave velocity lower than in the square lattice. Spatial properties of eigenmodes are characterized in several different ways. At low energies, eigenstates are relatively extended, and show multifractal scaling. At higher energies, states are more localized, and, depending on the energy, confined to sites of a specified coordination number. The ground state energy of this antiferromagnet, and local staggered magnetizations are calculated. Perpendicular space projections are shown, showing the underlying simplicity of this “complex” ground state. A simple analytical model, the two-tier Heisenberg star, is presented to explain the staggered magnetization distribution in this antiferromagnetic system.

9:36AM X13.00009 Loop Algorithm for the SU(N) Heisenberg Model . NAOKI KAWASHIMA, ISSP, University of Tokyo — The SU(N) generalization of the Heisenberg model is studied with a new loop algorithms with non-binary loop variables.[1] The split-spin representation is used for high-dimensional representations. While we have confirmed our previous result[3] that the ground state switches from the Neel state to the VBS state around N=5 for the fundamental representation, we also find that there is an apparent U(1) symmetry in the VBS state. For higher representation, we have not observed any VBS state, although the disappearance of the Neel order parameter has been detected as we increase N. [1] N. Kawashima and K. Harada, J. Phys. Soc. Jpn. 73 1397 (2004).

9:48AM X13.00010 Dynamical properties of SSH and breathing type Hamiltonians . HANS GERD EVERTZ, PETER PIPPAN, Techn. Univ. Graz — Using a QMC method based on exact phonon integration in Fourier space and on loop updates in particle space, we study fermionic systems coupled to dynamical phonons in one dimension. Within this method it is possible to investigate Su-Schrieffer-Heeger (SSH) as well as Holstein type models, with momentum dependent couplings (e.g. breathing phonons) and arbitrary phonon dispersions. We access the dynamical properties of the systems via momentum dependent phonon spectral functions and electron Greens functions. In case of the standard Holstein model, we present precise data for the phonon spectral function in both the metallic Luttinger liquid and the insulating charge density wave phase, for a wide range of phonon frequencies.

Friday, March 14, 2008 8:00AM - 11:00AM — Session X15 DBP FIAP: Emerging Nano-based Diagnostics and Therapeutics: Approaches to Cancer Treatment Morial Convention Center 207
8:00AM X15.00001 Intracellular Mechanics-Based Drug Screening for Cancer Metastasis, YILDER TSENG, University of Florida — In 2007 alone, close to 1.5 million new cancer cases and over half of a million deaths from cancer are projected to occur in US. In general, cancer is much easier to be successfully treated before metastasis; the five-year survival rates for most of the cancers in the metastatic stage are lower than 10%. The origin of cancer is due to genomic instability; however, the genomics or proteomics studies focus on this phenomenon cannot thoroughly elucidate how cancer metastasis proceeds. During this process, cancer cells protrude and conquer their physical barriers, resist shear stress, establish anchorage and finally settle in a new environment. Each development in this process involves mechanical forces. Thus, whether force generation and cancer cells' mechanical properties can be integrated into the current mainstream of cancer research and offer new insight is worthy of being investigated. To measure the change of cell mechanics, specifically intracellular mechanics, a tool that least disrupts the probed cell’s behavior and, simultaneously, can obtain real time quantitative measurement is necessary. To satisfy these criteria, we have developed a technique, ballistic intracellular nanorheology (BIN), in which we trace and analyze the trajectories of nanoparticles that have been ballistically bombarded into the cytoplasm of individual cells. This technique allows us to probe the effects of chemical or mechanical stimuli on intracellular mechanics in various types of cells, on culture dishes or in a three-dimensional matrix. BIN is currently, the first and only method available that can be applied to perform such tasks. Using this technique, we have gained detailed information about how the cytoskeletal remodeling pathways control the intracellular mechanics. We have also obtained information on the tempo-correlation between agonists and intracellular mechanics and how cells utilize their intracellular mechanics to react extracellular shear stress. These studies have set the framework for us to understand the mechanical mechanism of cancer cell metastasis on a molecular level. In this talk, I will describe the working principal using this technique to screen cancer drugs that prevent cancer metastasis.

8:36AM X15.00002 Targeted Multifunctional Nanoparticles cure and image Brain Tumors: Selective MRI Contrast Enhancement and Photodynamic Therapy, RAOUl KOPELMAN, University of Michigan — Aimed at targeted therapy and imaging of brain tumors, our approach uses targeted, multi-functional nano-particles (NP). A typical nano-particle contains a biologically inert, non-toxic matrix, biodegradable and bio-eliminable over a long period time. It also contains active components, such as fluorescent chemical indicators, photo-sensitizers, MRI contrast enhancement agents and optical imaging dyes. In addition, its surface contains molecular targeting units, e.g. peptides or antibodies, as well as a clamping agent, to prevent uptake by the immune system, i.e. enabling control of the plasma residence time. These dynamic nano-platforms (DNP) contain contrast enhancement agents for the imaging (MRI, optical, photo-acoustic) of targeted locations, i.e. tumors. Added to this are targeted therapy agents, such as photosensitizers for photodynamic therapy (PDT). A simple protocol, for rats implanted with human brain cancer, consists of tail injection with DNPs, followed by 5 min red light illumination of the tumor region. It resulted in excellent cure statistics for 9L glioblastoma. 3Thank you to the National Cancer Institute and the National Science Foundation, Division of Materials Research

9:12AM X15.00003 Microcantilever Biosensors, THOMAS THUNDAT, Oak Ridge National Laboratory — Micromachined cantilever beams respond to molecular adsorption by with mechanical bending. For small concentrations, the bending signal is directly proportional the surface concentration of adsorbed molecules. Selectivity in detection is accomplished by immobilizing specific receptors on one of the surfaces of the cantilever. We have developed microcantilever arrays for multiplexed, label-free detection of biomolecules. Photo-sensitive readout of cantilever bending offers a simple and rapid signal transduction that is compatible with microfabrication. Although the microcantilever-based biosensing appears to high sensitivity and selectivity, reproducibility of the technique appears to be a challenge. We have developed a novel method of immobilizing receptors that increases the reproducibility. We have demonstrated simultaneous detection of cancer and cardiac markers using cantilever arrays with immobilized receptors. We will also discuss a receptor-free mode of achieving selectivity.

9:48AM X15.00004 Magnetic sifters and biochips for early diagnosis and therapy monitoring of cancer, CHRIS EARHART, Stanford University — Magnetic nanoparticles conjugated with biomolecules or recognition moieties are finding wide applications in medicine. In this context, we are developing a micromachined magnetic sifter and magnetic nanoparticles aimed for sample preparation applications in early diagnosis of cancer. The microfabricated sifter consisting of arrays of micron sized slits etched through a silicon wafer. A magnetic film is deposited on the wafer, producing high magnetic field gradients, comparable in magnitude to gradients in planar flow devices. As the solution flows through the die, magnetic particles are captured by the magnetic material surrounding the slits. The large number of slits allows for processing of large volumes of liquid, much greater than that of planar microfluidic devices. The sifters can be simply attached to a syringe or tube, resulting in a portable and user-friendly tool for molecular biology. The separation efficiencies of ~ 50% for one pass through the sifter have been achieved. We have also designed and fabricated several types of magnetic biochips consisting of arrays of giant magnetoresistive (GMR) spin valve detectors with appropriate dimensions, surface chemistry, and microfluidics. An advanced electronic test station has been set up as a demonstration vehicle for the integrated evaluation of our magnetic biochips with commercial and custom magnetic nanoparticle labels for DNA or protein biomarkers. The magnetic biochip is capable of detecting down to 1-30 nanotags. Real-time detection of DNA signatures and protein targets in buffer and serum samples has been successfully performed in our laboratories, suggesting that magnetic biochips hold great promises for molecular diagnostics of cancer and other diseases. In collaboration with Chris M. Earhart, Wei Hu, Robert J. Wilson, Sebastian J. Osterfeld, Robert L. White, Nader Pourmand, and Shan X. Wang @ Stanford University. This work was supported by grants from NIH (1U54CA119367-01) and DARPA/Navy (N00014-02-1-0807).

10:24AM X15.00005 Microdevices for biomolecular detection and single cell analysis, SCOTT MANALIS, MIT — Recent advances towards developing biomolecular and single cell applications for a mass-based biosensor known as the suspended microchannel resonator (SMR) will be presented. In SMR detection, target molecules or cells flow through a vibrating suspended microchannel and are captured by receptor molecules attached to the interior channel walls. What separates the SMR from the existing resonant mass sensors is that the receptors, targets, and their aqueous environment are confined inside the resonator, while the resonator itself can oscillate at high Q in an external vacuum environment, thus yielding extraordinarily high sensitivity. This approach solves the problem of viscous damping that degrades the sensitivity of cantilever resonators in solution. We have achieved a resolution of approximately 1 femtogram (1 Hz bandwidth) which is represents an improvement of six order of magnitude improvement over a high-end commercial quartz crystal microbalance. This gives access to intriguing applications such as mass based flow cytometry, real-time monitoring of single cell growth, and the direct detection of protein biomarkers.

Friday, March 14, 2008 8:00AM - 11:00AM —
Session X18 DPOLY: Focus Session: Dynamics and Structures in Polymer Melts, Gels and Glasses Morial Convention Center 210
alkane squalane (C23) the rheological properties of alkanes of the same length but with different architecture. The simulations were done in the NVT ensemble using the reverse evidence that subdiffusive behaviour found in contradiction to the Rouse model is also caused by the excluded volume interaction. [1] J. Wittmer, H. Meyer, J. 23. The viscosity was calculated for different shear rates and compared with experimental values. Different structural parameters such as the mean end-to-end distance, the radius of gyration, and the angle of alignment of the molecules with the flow were studied as a function of the shear rate. [2] A.D. Enevoldsen et al., J. Chem. Phys. 126, 104703-10 (2007); 126, 104704-17 (2007). [3] F. Müller-Plathe et al., Phys. Rev. E, 59, 4894 (1998)

1Supported by Grant Nos. U.S. NSF DMR-0705974, FONDECYT 1060628, CONICYT, and the Danish Center for Scientific Computing.

8:48AM X18.00003 Theory of the effect of deformation on the relaxation and mechanical properties of polymer glasses . KANG CHEN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — Recently Saltzman and Schweizer have developed a statistical dynamical theory of segmental relaxation in deeply supercooled polymer melts by combining and extending methods of mode coupling, dynamic density functional and activated barrier hopping theories. The approach is built on the concept of a nanometer scale nonequilibrium free energy which quantifies dynamic localization due to interchain forces. We have now generalized this approach to treat quiescent relaxation, physical aging, and nonlinear mechanical properties in the nonequilibrium glass state. Applied stress weakens dynamical constraints in the effective free energy which accelerates alpha relaxation and softens the elastic modulus. A constitutive equation has been constructed which allows the prediction of dynamic yielding and mechanical response under constant strain rate, constant stress (creep), and other modes of deformation. Multiple predictions that fundamentally differ from the phenomenological Eyring model are made for the temperature and strain rate dependence of the dynamic yield stress and the deformation modified segmental relaxation time. Comparison of the theoretical results with experiments on PMMA reveals good agreement. The coupling of stress and aging, the strain softening effect, and large deformation strain hardening, can also be treated within our approach.

9:00AM X18.00004 Why Temperature Variation of the Chain Relaxation is Universal for Many Polymers? . ALEXEI SOKOLOV, The University of Akron, UNIVERSITY OF AKRON TEAM — Temperature variations of chain and segmental modes are traditionally described through corresponding friction coefficients. It is usually assumed that the same friction mechanism controls dynamics of both processes. As a result, their temperature dependence is expected to be the same. It is known, however, that segmental relaxation in many polymers varies faster than the chain one when temperature approaches Tg. We present an analysis of temperature variations of segmental and chain modes for different polymers. We demonstrate [1] that the chain relaxation shows universal temperature dependence for many polymers when it is presented vs Tg/T. Even polymers with strongly different temperature behavior of segmental dynamics (fragility) exhibit the same behavior for the chain relaxation. These results indicate complete decoupling in behavior of chain and segmental modes and emphasize our deficiency in understanding the microscopic mechanism of the chain friction coefficient. Possible mechanisms that lead to so universal behavior of chain relaxation are discussed at the end.

8:00AM X18.00001 Elastomeric Photopolymers: Shaping Polymer Gels with Light . JULIA KORNFIELD, California Institute of Technology, Division of Chemistry and Chemical Engineering — Polymer gels that possess a latent ability to change shape, which can be triggered in a spatially resolved manner using light—“elastomeric photopolymers”—have been developed to meet the need for materials that can be reshaped without direct contact, e.g., to non-invasively adjust an implanted lens in the human eye. The physics of diffusion and swelling in elastomers are applied to create a transparent silicone suitable for making a foldable intraocular lens that can be reshaped using near ultraviolet light. A crosslinked silicone network dynamics. The approach is built on the concept of a nanometer scale nonequilibrium free energy which quantifies dynamic localization due to interchain forces. We have now generalized this approach to treat quiescent relaxation, physical aging, and nonlinear mechanical properties in the nonequilibrium glass state. Applied stress weakens dynamical constraints in the effective free energy which accelerates alpha relaxation and softens the elastic modulus. A constitutive equation has been constructed which allows the prediction of dynamic yielding and mechanical response under constant strain rate, constant stress (creep), and other modes of deformation. Multiple predictions that fundamentally differ from the phenomenological Eyring model are made for the temperature and strain rate dependence of the dynamic yield stress and the deformation modified segmental relaxation time. Comparison of the theoretical results with experiments on PMMA reveals good agreement. The coupling of stress and aging, the strain softening effect, and large deformation strain hardening, can also be treated within our approach.

8:36AM X18.00002 Dynamics of Swollen Gel Layers Anchored to Solid Surfaces . GEORGE FYTAS, FORTH, University of Crete, Greece, MARIA GIANNELI, University of Crete, Greece, ROBERT ROSKAMP, ULRICH JONAS, KALOIAN KOYNOV, WOLFGANG KNOLL, MIPIP Mainz, Germany, BENOIT LOPPINET, FORTH, Greece — Thin responsive hydrogel films are currently under development for biosensor applications. Photocrosslinkable poly(N-isopropylacrylamide) (PNIPAAm) based chains are spin coated as thin films (about 1 micron) and UV irradiated with variable doses to control the crosslink density. The obtained anchored gel layers can swell in ethanol or water up to about 10 microns for low crosslinking densities. Dynamics of the swollen layers and diffusion of different tracers (as analyte mimics) are studied by dynamic light scattering (PCS) and fluorescence correlation spectroscopy (FCS). PCS resolved fast and slow diffusions, attributed to cooperative diffusion and long range concentration heterogeneities. Higher crosslink densities give rise to faster cooperative diffusion, i.e. short dynamic mesh sizes. FCS revealed the importance of electrostatic interactions between probe and negatively charged network. While a negatively charged dye senses local dynamics with a moderate slow down, a positively charged dye exhibited substantially retarded diffusion. Larger tracers are used to assess the size dependent gel penetrability, whereas large particles, trapped into the network, expectedly follow the network dynamics.

12:00PM X18.00005 Molecular dynamics simulations of layers of linear and branched alkanes under shear . P. SOZA, P.U. Catolica Chile, F.Y. HANSEN, Tech. Univ. of Denmark, H. TAUB, U. Mo.-Columbia, U.G. VOLKMANN, P.U. Catolica Chile — We have previously studied the equilibrium structure and dynamical excitations in films of the linear alkane tetracosane (n-C24H50) and the branched alkane squalane (C30H62) in great detail. Here we report the results of nonequilibrium molecular dynamics simulations of these systems in order to compare the rheological properties of alkanes of the same length but with different architecture. The simulations were done in the NVT ensemble using the reverse nonequilibrium algorithm proposed by F. Müller-Plathe et al. The viscosity was calculated for different shear rates and compared with experimental values. Different structural parameters such as the mean end-to-end distance, the radius of gyration, and the angle of alignment of the molecules with the flow were studied as a function of the shear rate. A.D. Enevoldsen et al., J. Chem. Phys. 126, 104703-10 (2007); 126, 104704-17 (2007). [3] F. Müller-Plathe et al., Phys. Rev. E, 59, 4894 (1998)

8:24AM X18.00006 On the influence of excluded volume in polymer melts . HENDRIK MEYER, J.P. WITTMER, J. FARAGO, A. JOHNER, J. BASCHNAGEL, ULP Institut Charles Sadron, CNRS UPR22, Strasbourg, France — Flory’s ideality hypothesis states that polymer chains in the melt have random walk like conformations as if there would be no excluded volume. However, it was shown recently that the excluded volume interaction induces corrections to scaling which are long range and which give rise to a power law decay of bond-bond correlation function [1] as well as to corrections to the Kratky plateau of the form factor [2]. In this presentation, we focus on the Rouse mode analysis by switching on the excluded volume potential gradually to study the crossover from phantom chains (representing perfect random walks described by the Rouse model) to real polymer melts [3]. In the melt, significant corrections have to be made to the static Rouse mode spectrum and consequences for the dynamics are briefly discussed. This gives also evidence that subdiffusive behaviour found in contradiction to the Rouse model is also caused by the excluded volume interaction. [1] J. Wittmer, H. Meyer, J. Baschnagel et. al. Phys. Rev. Lett. 93 (2004) 147801. Phys. Rev. E 76 (2007) 011803. [2] J. Wittmer et. al. EPL 77 (2007) 56003. [3] H. Meyer et. al. accepted at Eur. Phys. J. E (2007)
9:36AM X18.00007 Observation of Anomalous Viscosity in Entangled Polymer Films near the Glass Transition  . ZHANG JIANG, Dept. of Physics, University of California at San Diego & Advanced Photon Source, ANL, M. K. MUKHOPADHYAY, SUNIL K. SINHA, Dept. of Physics, University of California at San Diego, SURESH NARAYANAN, Advanced Photon Source, ANL, LAURENCE B. LURIO, Dept. of Physics, Northern Illinois University, SANGHOON SONG, HYUNJUNG KIM, Dept. of Physics & Interdisciplinary Program of Intergrated Biotechnology, Sogang University, Korea — We have studied the viscous relaxation of surface waves on molten polystyrene films of various molecular weights ($M_w$) using x-ray photon correlation spectroscopy. The relaxation time has been measured as a function of wave vector from high temperatures down to near the bulk glass transition temperature ($T_g$). We find a transition from a single exponential regime through a stretched exponential to another single exponential regime with increasing temperature. The transport dynamics of polymer films at $T_g$ where the effective viscosity saturates at that of chains with critical molecular weight for entanglement. These results are interpreted in terms of the freezing-out of relaxation modes involving full chains and large segments until only fluctuations of chain segments of critical entanglement length survive. We also find no evidence for a low viscosity surface layer near $T_g$.

9:48AM X18.00008 Kohrausch Parameter Determination for Simple Chain Models  . JOHN MCCOY, TAYLOR DOTSON, JULIENNE HEFFERNAN, KEENAN DOTSON, Materials Department, New Mexico Tech, Socorro, NM 87801, JOANNE BUDZIEN, DOUGLAS ADOLF, Sandia National Laboratories, Albuquerque, NM 87185 — The second Legendre polynomials of the end-to-end vector of freely jointed and freely rotating chains were extracted from molecular dynamics simulations and analyzed in terms of the Kohrausch-Williams-Watts (KWW) function. Of particular interest is the variation of the stretching exponent, $\beta$, as a function of state point and, consequently, of the detailed compliance with time-temperature superposition. A new analysis methodology is introduced that permits the determination of $\beta$ at the needed level of precision. Detailed time-temperature superposition does not hold for freely-jointed or freely-rotating chain liquids. Indications of a breakdown in time-temperature superposition are also found in violations of Stokes-Einstein and Debye-Stokes-Einstein behavior.

10:00AM X18.00009 Understanding Fragility in Polymers  . KUMAR KUNAL, The University of Akron, CHRISTOPHER ROBERTSON, Bridgestone Americas Center for Research and Technology, ALEXEI SOKOLOV, The University of Akron, THE UNIVERSITY OF AKRON TEAM, BRIDGESTONE AMERICAS CENTER FOR RESEARCH AND TECHNOLOGY COLLABORATION — Glass transition in polymeric liquids is an important phenomenon that still remains poorly understood. It is accompanied by strongly non-Arrhenius temperature variations of segmental relaxation time $\tau_\alpha$. The deviations of $\tau_\alpha$ from Arrhenius behavior is described by the fragility parameter, $m$: $m = \beta \log (\tau_\alpha/(T-T_g))/\tau_\alpha T_g$, where $T_g$ is the glass transition temperature. It appears that polymers are very fragile compared to small molecular weight liquids. However, there are some polymers that have intermediate fragility too. The reason for high fragility of polymers remains a topic of active discussion. We have studied various polymer systems using dielectric spectroscopy and dynamic mechanical analysis, and present an analysis of the results in the framework of chain flexibility, symmetry of the monomer and the packing efficiency of the polymer melt.

10:12AM X18.00010 Dye Reorientation as a Probe of Stress-induced Mobility in PMMA Glasses  . HAU-NAN LEE, University of Wisconsin-Madison, KEEWOOK PAENG, STEPHEN SWALLEN, MARK EDIGER — To understand the response of molecular glasses to deformation, we perform optical measurements of dye reorientation in PMMA glasses under stress. The reorientation of probes can be used to monitor the segmental dynamics of a polymer melt. We utilize this method to quantitatively determine the stress-induced mobility in PMMA glass during tensile creep deformation. At 377 K ($T_g$-18 K), a stress of 20 MPa accelerates the mobility by a factor of 100, while 11 MPa has almost no effect. After removing the stress, we observe that the enhanced mobility slowly disappears, even though the overall strain is still very large.

10:24AM X18.00011 On the effect of Molecular weight and Frequency dependence of $T_g$ on the interpretation of Dynamic viscosity data  . J.P. IBAR, Un. de Pau URM256, Pau 64013, A. ALLAL UNIV. DE PAU 64013 COLLABORATION — In this work, we re-plot dynamic data for a series of monodispersed Polystyrene melts, and their blends, obtained at constant temperature and variable frequency $\omega$, to enable a new analysis at constant ($T-T_g$) instead, where $T_g$ is made a function of $M_n$ and $\omega$. $T_g$ ($\omega$) is determined by DMA, from the shift of the max of $E''$ with $\omega$. $T_g$ increases rapidly with $\omega$ and levels off at higher $\omega$. The $M_n$ dependence of $T_g$ varies in a similar way, quickly plateaus off at approximately $M_n$=2 Me, consistent with a free volume interpretation. It is shown that correction for the $T_g$ dependence on $M_n$ and $\omega$ does play an important role in the determination of the scaling parameters exponents, such as the molecular weight dependence exponent for $M_n$=2 Me data, or the low frequency tail representative of the terminal behavior for blends of monodispersed samples. The paper concludes that a true separation of the variables to determine the independent effect of structural (local) and molecular weight (scaling) factors, can only be done at constant ($T-T_g$). The incidence of $T_g$($\omega$, $M_n$) on the superposition at low $\omega$, is also reviewed.

1 work supported by Fulbright Grant.

10:36AM X18.00012 Influence of pressure (density) on fast dynamics in polymers  . LIANG HONG, BURAK BEGEN, ALEXANDER KISLIUK, ALEXEI SOKOLOV, University of Akron, DR SOKOLOV'S GROUP TEAM — Understanding the microscopic nature of the fast dynamics in disordered materials is still a challenge. In particular, the origin of the collective vibrations, the so-called Boson peak, remains a subject of active discussion. It’s known that Boson peak spectra change significantly under pressure. Analysing the role of density in the Boson peak might help to unravel its microscopic nature. In this work, we use light scattering to study influence of pressure (up to 1.5 GPa) on fast dynamics in different polymers. In all cases, the observed shift of the Boson peak frequency with pressure is significantly stronger than change of sound velocities. This result clearly indicates that elastic continuum approximation cannot describe the pressure-induced variations. We demonstrate that the main variation of the Boson peak amplitude is due to changes of the Debye level, although detailed quantitative analysis is not possible due to the light-to-vibration coupling coefficient, which also varies with pressure. Analysis also shows there is a correlation between pressure-induced changes in the Boson peak frequency and amplitude.

10:48AM X18.00013 Visualization and Analysis of the Dynamics of Methanol Transport in Poly(Methyl Methacrylate)  . ADAM EKENSEAIR, RICHARD KETCHAM, NICHOLAS PEPPAS, The University of Texas at Austin — The relative rates of the diffusional and relaxational processes during the absorption of penetrating molecules in glassy polymers determine the nature of the transport process and lead to a myriad of transport phenomena, such as Fickian, Case II, and anomalous absorption behavior. Many proposed models account for the majority of anomalous behavior that has been observed. However, there is still a disconnect between theory and experiment, as data must be fit to the model and adjustable parameters determined. We propose that a better understanding of the dynamics of penetrant transport in glassy polymers can be achieved by careful and detailed investigations into the role the polymeric network structure plays in influencing the transport mechanism. We introduce a novel technique to visualize and quantify transport dynamics and mechanisms in situ. High-resolution X-ray computed tomography, a completely nondestructive technique that can be used to visualize features in the interior of opaque solids, has been successfully adapted to examine the transport dynamics of methanol into glassy poly (methyl methacrylate) discs synthesized by an infusion-mediated free radical polymerization. In addition to tracking methanol absorption and dimensional swelling, the time-dependent concentration profiles within the polymer disc were determined.
8:00AM X22.00001 Ab initio simulations of the transport properties of Mn$_{12}$ based spin-devices . CHAITANYA DAS PEMMARAJU, IVAN RUNGGER, STEFANO SANVITO, Trinity College Dublin, Ireland, COMPUTATIONAL SPINTRONICS GROUP, TCD TEAM . Single-molecule magnets (SMMs) represent a unique playground for fundamental quantum physics and exhibit exotic phenomena such as magnetic hysteresis as well as magnetization reversal through quantum tunneling . Recently, transport measurements on Mn$_{12}$ based molecular magnets in single-molecule-transistor devices have been realized . In this work we present ab initio transport[1] calculations of Mn$_{12}$ molecules functionalized by thioether groups and sandwiched between gold contacts . We find the transport properties of these SMMs to be dominated by tunneling type behaviour across the organic functional groups and asymmetric coupling to the leads . We observe asymmetric I-V curves under positive and negative bias . In addition we demonstrate that the I-V characteristic changes upon changing the magnetic state of the molecule, suggesting that electrical single-spin detection can be indeed obtained from a detailed knowledge of the I-V .

1] Rocha et. al, Spin and Molecular Electronics in an Atomically Generated Orbital Landscape; URL: http://www.smeagol.tcd.ie

8:12AM X22.00002 Modeling the organic magnet Fe[TCNE]$_2$ . J. MORENO, M.A. MAJIDI, University of North Dakota, K.I. POKHODNYA, North Dakota State University — Recent experiments have revealed the crystal structure of Fe[TCNE]$_2$ , (TCNE = tetracyano-ethyleno), an organic-based magnet with a transition temperature around 100 K and a saturation magnetization corresponding to an effective spin of 3/2 per formula unit . Its structure consists of undulating layers of TCNE anion-radicals bound to four Fe(II) ions, where Fe ions between adjacent layers coupled via diamagnetic σ-dimerized TCNE . Since the angular momentum of Fe(II) is almost quenched due to the asymmetric crystal field, we model the system using a Heisenberg Hamiltonian with antiferromagnetic in-plane coupling between the Fe(II) S=2 spins and the near-neighbor (TCNE) S = 1/2 spins and also antiferromagnetic superexchange coupling between the Fe(II) spins at adjacent planes . By comparing our results with magnetization measurements as function of temperature and field, we extract the values of the inter- and intra-plane antiferromagnetic couplings . We discuss how to extend our approach to other TCNE-based magnets, such as the amorphous semiconducting V[TCNE]$_2$ , a room temperature ferrimagnet and promising candidate for multifunctional spintronic applications .


8:24AM X22.00003 Reversible Photoinduced Magnetism in V-Cr Prussian blue analogues . K. DENIZ DUMAN, JUNG-WOO YOO, N.P. RAJU, Physics, The Ohio State University, AMBER C. MCCONNELL, WILLIAM W. SHUM, KENDRIC J. NELSON, JOEL S. MILLER, Chemistry, University of Utah, A.J. EPSTEIN, Physics and Chemistry, The Ohio State University — The cyan-o-bridged bi-metallic compounds, so called “Prussian blue magnets,” display a broad range of interesting photoinduced magnetic phenomena . A notable example is Fe-Co Prussian blue magnet, which exhibits light-induced changes in between magnetic states together with glassy behavior[1,2] . Here, we report reversible photoinduced magnetic phenomena in V-Cr Prussian blue analogue (K$_{1.54}$V$_{0.65}$Cr(CN)$_{6}$)(SO$_{4}$)$_{0.13}$3.1H$_2$O, one of the few room temperature molecule-based magnets . Illumination with UV light suppresses magnetization, whereas subsequent illumination with green light increases magnetization . This recovery effect of green light is observed only when the sample is previously UV-irradiated . This suggests a hidden metastable magnetic state with a long lifetime at low T (<100 K) . Results of detailed magnetic studies and the likely microscopic mechanisms will be discussed . [1] Hashimoto et al. science 272, 5262 (1996); [2] Pejakovic, et al. PRL 85 1994 (2000)

8:36AM X22.00004 Magnetic properties of organic-based Ni[TCNE](MeCN)$_2$[BF$_4$] magnet . KONSTANT IN POKHODNYA, CNSE NDSU, Ohio State University; University of Utah, VICTOR DOKUKIN, JOEL S. MILLER, University of Utah — A new organic-based magnet Ni[TCNE](MeCN)$_2$[BF$_4$] (1 composite-hyphenylene) was synthesized via reaction of NiBr$_2$(TCNE) and Ni(NCMe)$_2$(BF$_4$)$_3$ in CH$_2$Cl$_2$ . Zero field cooled and field cooled magnetizations, M(T)$_{ZFC}$ and M(T)$_{FC}$, at 0.5 mT rise sharply below 70 K indicative of an onset of a magnetic transition . M(T)$_{ZFC}$ reaches maximum at 25 K followed by a rapid decrease suggesting antiferromagnetic (AF) interaction . In contrast, M(T)$_{FC}$ rises upon further cooling signifying a strong irreversibility in accord with sharp increase of a remanant magnetization below 30 K and hysteretic behavior of M(H) . The M(H) at 2 K increases rapidly with field and approaches saturation above ~ 0.5 T . At 9 T M(H) reaches 2.24 $\mu_B$/molecule that is significantly higher than 1.30 $\mu_B$ expected for AF coupled Ni(II) S = 1 and [TCNE]$^-$ (S = 1/2) suggesting a ferromagnetic (FM) interaction . The unpaired Ni$^{2+}$ spins and those on the [TCNE]$^-$ reside in orthogonal orbitals resulting in FM coupling . Assuming that similarly to Fe[TCNE][FeCl$_2$(MeCN)$_2$] 1 consists of Ni$^{2+}$ - μ$_{Fe}$-[TCNE]$^-$ layers we believe that the decrease of M(T)$_{ZFC}$ below 25 K is due to AF coupling between the layers while the interaction within the layer is FM in contrast to the AF one reported for Fe, V, and Mn analogues .

Supported in part by DOE (DE-FG03-93ER45504, DE FG 02-86BR45271 and DE-FG02-01ER45831) and AFOSR (F49620-03-10175) and NSF ND EPSCoR EPS-0447679 grants.

8:48AM X22.00005 Magnetoresistance in bulk heterojunction solar cells . RONALD OESTERBACKA, Abo Akademi University, SAYANI MAJUMDAR, University of Turku, HIMALDRI MAJUMDAR, HARRI AARNIO, Abo Akademi University, REINO LAIHO, University of Turku — The magnetoresistance (MR) response of the poly(3-hexyl thiophene) and poly(3-hexyl thiophene):1-(3-methoxy carbonyl) propyl-1-phenyl-[6,6]-methanofullerene (PHT:PCBM) based bulk heterojunction solar cells have been studied . Positive MR was always observed at room temperature in both the devices . In both cases the magnitude of the MR signal decreases at lower temperature and shows positive to negative sign inversion at 100K for the solar cells and at 200K for P3HT . The detailed voltage and temperature dependence of MR will be presented which will give important insight of the magnetic field effect on the bulk carrier mobility in the organic solar cells . We have observed tendency of retaining magnetic history in both the devices and it has been studied .

9:00AM X22.00006 Extending transfer-matrix studies of charge transport in dsDNA: diagonal ladder model . STEPHEN WELLS, RUDOPH ROEMER, University of Warwick — The π-stacking of aromatic bases along the axis of the DNA double helix suggests that DNA should be capable of supporting electron transport . This possibility has been investigated by a variety of experimental methods, including charge-transfer between intercalated dye molecules and direct measurement of conductivity in DNA molecules bridging two electrodes . In order to explore either the biological or nanotechnological significance of charge transport in DNA, we need theoretical models capable of predicting the influence of DNA sequence and structure on its charge transport properties . Transfer matrix methods have been used in conjunction with a ladder model of dsDNA (incorporating charge transfer between adjacent bases along a strand, and between hydrogen-bonded base pairs) to predict different transport properties for random, repetitive, or coding DNA sequences . It has been suggested that DNA charge transport may be involved in cellular mechanisms to detect and repair damage to DNA strands . We present extensions to the ladder model to allow for, firstly, charge transfer “diagonally” (from a base on a 5’ strand to an adjacent base on a 3’ strand, for example), and secondly, variations in hopping amplitudes due to bending of the helix (for example, in wrapping round a histone complex) . Hence we take into account the extent of the electronic states and the geometry of the DNA strand in our modeling .
9:12AM X22.00007 Sequence Dependent Charge Transport on Double Stranded DNA1, EFTA YUDIARSAH, SERGIO E. ULLOIA, Ohio University — The transport properties of different double-stranded DNA sequences are studied by transfer and scattering matrix methods. The DNA is described by a tight-binding model with realistic sequence-specific hopping integrals. Our results show that, in qualitative agreement with experimental results [1], even a single base mismatch on the sequence can dramatically change the conductance of short DNA sequences. The change in conductance is larger if the mismatch is on the energetically favorable path of transmission: the path with the most bases with energy close to the Fermi energy of the contacts. This trend is independent on which strand is being connected to the electrodes, although similar sequences have drastically different conductance values. We also study the effect of structural “nicks” on the DNA conductance. In accordance with experimental results [2], the conductance is changed by several orders of magnitude in the presence of the nicks, depending on the position of the defect on the strand. As the conductance of a strand is found to be dependent on the sequence of bases, this suggests an electronic approach to sequencing [1]. [1] J. Hihath et al., Proc. Natl. Acad. Sci. U. S. A. 102, 16979 (2005). [2] B. Hartzel et al., Appl. Phys. Lett. 82, 4800 (2003).

1Supported by OU-BNNT

9:24AM X22.00008 Theory of electron conductance across a DNA basepair, MYEONG LEE, OTTO SANKEY, Arizona State University — In recent years, research on electron tunneling through DNA basepairs has become more important due to its potential application in DNA sequencing technology. The goal is to recognize and identify a specific DNA base by measuring the hydrogen bond mediated tunneling current across a DNA base pair junction. In this talk, we discuss the results of density functional theory in the intrinsic conductance through DNA basepairs (Watson-Crick base pairs, Wobble base pairs, etc), and in particular the role of the hydrogen bond on the tunneling current.

9:36AM X22.00009 Charge transport in guanine crystals, FRANK ORTMANN, KARSTEN HANNEWALD, FRIEDHELM BECHSTEDT, ETSF and IFTO, Friedrich Schiller University Jena, Germany — Charge-transport processes in organic molecular crystals exhibit similarities and differences to those in r-conjugated polymers. For both types of condensed matter the polaronic effects are of high importance. These effects can cause a transition from bandlike transport to thermally activated hopping. While the hopping regime is prevalent for DNA polymers, it is not clear if the same holds also for crystalline guanine or if band transport dominates. Also the influence of the temperature is rarely discussed in literature. In our approach to the problem of charge-carrier transport in these systems [1], we discuss the temperature dependence of the polaron bandwidth and the mobility in guanine crystals [2].


Friday, March 14, 2008 8:00AM - 10:48AM —
Session X23 DMP MAG: Focus Session: Multiferroics III: Other —
Morial Convention Center 215

8:00AM X23.00001 Pyroxenes: A novel class of multiferroics1, 2, D.J. KHOWSKII, Koeln University, S. JODLAU, P. BECKER, J. MYDOSH, TH. LORENZ, S.V. STREITSLSOV, D.C. HEZEL, L. BOHATY — Pyroxenes with the general formula AMSi2O6 (M = mono- or divalent metal) are shown to be a new class of multiferroic materials. In particular, we have found so far that NaFeSi2O6 becomes ferroelectric in a magnetically ordered state below 6 K. Similarly, magnetically driven ferroelectricity is also detected in the Li homologues, LiFeSi2O6 (Tc = 18 K) and LiCs2Si2O6 (Tc = 11 K). In all these monoclinic systems the electric polarization can be strongly modified by magnetic fields. Measurements of magnetic susceptibility, polarization current and dielectric constants (and their dependence on magnetic field) are performed using a natural crystal of aegirine (NaFeSi2O6) and synthetic crystals of LiFeSi2O6 and LiCs2Si2O6 grown from melt solution. For NaFeSi2O6 a temperature versus magnetic field phase diagram is proposed. Exchange constants are computed on the basis of ab initio band structure calculations. The possibility of a spiral magnetic structure caused by frustration as origin of the multiferroic behaviour is discussed. We propose that other pyroxenes may also be multiferroic, and that the versatility of this family offers an exceptional opportunity to study general conditions for and mechanisms of magnetically driven ferroelectricity.


8:12AM X23.00002 Magnetic field induced ferroelectricity in Mn11.9Fe0.1WO4, RAJIT CHAUDHURY, BERND LORENZ, YAQI WANG, YANYI SUN, CHING-WU CHU, TCSUH and Department of Physics, University of Houston, Houston, Texas 77204-5002, USA — We discovered the external magnetic field induce ferroelectric phase in Mn11.9Fe0.1WO4, which is paraelectric at zero magnetic field. The ferroelectric phase appears in fields above 4 Tesla applied along the easy axis of magnetization and the spontaneous polarization along the b-axis was measured by the pyroelectric method as a function of temperature and magnetic field. The temperature and magnetic field dependence of spontaneous polarization shows strong coupling between magnetic and ferroelectric orders. We interpret that the improper ferroelectricity in this compound is driven by non collinear spin structure which breaks the inversion symmetry. We propose high-field neutron scattering experiments to characterize the magnetic structure in the ferroelectric phase.

8:24AM X23.00003 Quantum theory of multiferroics in quasi-one-dimensional spin-1/2 frustrated magnets1, SHIGEKI ONODA, MASASHIRO SATO, RIKEN (Institute of Physical and Chemical Research), Wako 351-0198, Japan, YASUHIRO SAIGA, Department of Physics, Nagoya University, Nagoya 464-8602, Japan, SHUNSUKU FURUKAWA, RIKEN (Institute of Physical and Chemical Research), Wako 351-0198, Japan — A theory is developed to understand recent experimental findings on quasi-one-dimensional spin-1/2 multiferroics LiCuVO3 and LiCu2O2. For this purpose, weakly coupled frustrated quantum spin chains with and without the zigzag structure are studied by means of an effective field theory based on the bosonization in one dimension. A chiral ground state with gapless incommensurate spin excitations can be stabilized in the presence of an easy-plane anisotropy. This state is driven by a three-dimensional coupling to the incommensurate helimagnetic state, in accordance with the experimental observations. We also reveal the quantum dynamics of the spin, the chirality and the electromagnon as well as the finite-temperature phase diagram, which reflect the one-dimensional nature of the quantum fluctuations.

1The work is partly supported by the Grant-in-Aids from the Japan Society for the Promotion of Science.

8:36AM X23.00004 Correlation between spin helicity and electric polarization vector in quantum chain magnet LiCu2O2, SHINICHIRO SEKI, YUICHI YAMASAKI, YOSHINORI TOKURA2, Department of Applied Physics, University of Tokyo, MINORU SODA, MASATO MATSUURA, KAZUMA HIROMA, The Institute for Solid State Physics, University of Tokyo — Measurements of polarized neutron scattering were performed on the multiferroic quantum chain magnet LiCu2O2. In the ferroelectric ground phase, the existence of transverse spiral spin component in the bc-plane was confirmed. When the direction of electric polarization is reversed, the vector spin chirality as defined as Cij = S1 × S2 is also reversed. This directly proves that the spin-current model Pij ∝ eij × Cij is applicable even to this eij-electron quantum S=1/2 system. Differential scattering intensity of polarized neutrons shows a large discrepancy from that expected for the classical bc-cycloidal spin structure, implying either the complexity of magnetic structure or the effect of quantum fluctuation.

1also at Multiferroics Project, ERATO, Japan Science and Technology Agency (JST)
8:48AM X23.00005 Multiferroics versus Quantum Fluctuations in Spin-1/2 Frustrated Chains
 SHUNSUKÉ FURUKAWA, MASAHIRO SATO, SHIGEKI ONODA, RIKEN — We study interplay of the chiral spin ordering and quantum fluctuations in a spin-1/2 frustrated chain, which is the simplest model for one-dimensional multiferroic cuprates like LiCuVO$_4$ and LiCu$_2$O$_2$. In a Heisenberg chain, it is known that the classical helical magnetic order is suppressed by strong quantum fluctuations and valence-bond solid phases emerge. In fact, weak easy-plane spin anisotropies exist in the above materials, because of the XXZ-type anisotropy and a phonon-induced biquadratic Dzyaloshinskii-Moriya interaction. In particular, when the nearest-neighbor exchange coupling is much weaker than the antiferromagnetic second-neighbor one, our exact-diagonalization calculations combined with the bosonization analyses show that such anisotropies bring about the vector-chiral spin ordering and the associated multiferroic behavior. This chiral state is accompanied by slightly incommensurate algebraic spin correlations, which, with a three-dimensional coupling, explains the magnetic order experimentally observed in LiCuVO$_4$.

9:00AM X23.00006 Optical spectroscopic study on magnetoelectric MnWO$_4$. WOO SEOK CHOI, Seoul National University, KOUJI TANIGUCHI, Tohoku University, SOON JAE MOON, SUN JUNG KIM, SUNG SEOK A. SEO, Seoul National University, YOON SANG LEE, Soongsil University, TAKA-HISA ARIMA, Tohoku University, TAE WON NOH, Seoul National University — We report optical spectroscopic investigation on a multiferroic oxide compound, MnWO$_4$. This compound is known to exhibit ferroelectricity induced by the incommensurate spiral magnetic ordering in a temperature range of 7.6 K and 12.7 K [1]. We grew single crystals of MnWO$_4$ by using the floating zone method. To examine the optical anisotropy originating from the monoclinic crystal structure, we measured reflectivity spectra of MnWO$_4$ with light polarizations along three crystallographic axes, and calculated the optical conductivity spectra through the Kramers-Kronig transformation for each axis. We discuss the anisotropic phonon structures and electronic structures with temperature and magnetic field dependence in relation to its multiferroic properties.

9:00AM X23.00007 Ferroelectric domain topology of the multiferroic spin spiral system MnWO$_4$. D. MEIER, TH. LOTTERMOSER, G. YUAN, M. FIEBIG, HISK P - Univ. Bonn, Germany, P. BECKER, L. BOHATY, Institute of Crystallography, Univ. Cologne, Germany — The strong interest in magnetoelectric multiferroics is due to their potential concerning the design of novel multifunctional devices, as well as to their unusual physical properties. Among these, Tb$_2$Mn$_2$O$_7$, Ni$_2$V$_2$O$_8$, and MnWO$_4$ form a particularly challenging group: The key factor for ferroelectricity lies in the long-wavelength magnetic order. Many aspects of the precise nature of the ferroelectric state in such a spiral magnet, and in particular their coupling to the magnetic order, are still largely unclear. Here we report about the three-dimensional spatial distribution of ferroelectric domains in MnWO$_4$, revealed by optical second harmonic generation (SHG). Although ferroelectricity is induced by cycloidal spiral magnetic order, 180° domains as in a conventional ferroelectric are observed. Their coupling to the coexisting magnetic order and modifications of this coupling by external parameters such as temperature variation are discussed using spatially resolved SHG for probing both the magnetic and the ferroelectric order in one experimental run.

9:00AM X23.00008 Magnetic field control of the ferroelectric polarization in multiferroic MnWO$_4$. KOUJI TANIGUCHI, NOBUYUKI ABE, TAKAHIWA ARIMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, TAISHI TAKENOBU, YOSHIHIRO IWASA, Institute for Materials Research, Tohoku University — The relationship between magnetic order and ferroelectric properties has been investigated for MnWO$_4$. Spontaneous electric polarization is observed in a cycloidal spiral spin phase. The magnetic-field dependence of electric polarization indicates that the noncollinear spin structure plays a key role for the appearance of ferroelectric phase. Destabilization of the ferroelectric phase and an electric polarization flop from the b direction to the a direction have been observed when a magnetic field is applied along the b axis. On the other hand, the ferroelectric phase is stabilized when a magnetic field is applied along the a, c- and the spin easy axes. We have also found that the magnetic field induced ferroelectric polarization disappears in a high magnetic field above $12T$ along the spin easy axis. These phenomena provide us useful information for giant magnetoelectric effects because MnWO$_4$ is a simple system without rare-earth f-moments.

9:36AM X23.00009 Ferroelectricity in Mn$_{0.9}$Fe$_{0.1}$WO$_4$ induced by magnetic fields: A simple model calculation. B. LORENZ, R. P. CHAUDHURY, C. W. CHU, TCSUH and Department of Physics, University of Houston — Replacing Mn$^{2+}$ by Fe$^{3+}$ in multiferroic MnWO$_4$ results in the complete loss of ferroelectricity at zero magnetic field. However, it was shown that in Mn$_{0.9}$Fe$_{0.1}$WO$_4$ an external magnetic field restores the ferroelectric state. We present a simple mean field calculation of the Heisenberg model with ferromagnetic nearest and antiferromagnetic next nearest neighbor interactions and uniaxial anisotropy in an external magnetic field. The various commensurate and incommensurate magnetic phases in Mn$_{0.9}$Fe$_{0.1}$WO$_4$ with increasing Fe substitution is explained by the enhancement of the anisotropy. We show that the external field does indeed restore the helical spin structure in Mn$_{0.9}$Fe$_{0.1}$WO$_4$ and that the observed field-induced ferroelectricity can be explained.

9:48AM X23.00010 Correlation between magnetic, dielectric phase and strain in a Mn$_3$O$_4$ single crystal. T. SUZUKI, KATSUFUJI, Dept. of Physics, Waseda University — Mn$_3$O$_4$ has a tetragonal distorted spinel structure below 1443 K and exhibits a ferrimagnetic ordering at $T_N = 43$ K. This compound exhibits further magnetic phase transitions at 39 K and 33 K, where Mn$^{2+}$ and Mn$^{3+}$ spins are cantled from the collinear spin structure. We measured the dielectric constant and strain of a Mn$_3$O$_4$ single crystal. We found that both dielectric constant and strain have clear anomalies at the magnetic transition temperatures. We also found that dielectric constant is suppressed (enhanced) by 2% when magnetic field is applied parallel (perpendicular) to the direction of electric field within the $ab$ plane below $T_N$. In addition, strain along the $ab$ plane also has anisotropic magnetic field dependence. These results can be explained as follows: (1) There is an orthorhombic distortion below $T_N$, presumably induced by the orbital ordering of Mn$^{3+}$; (2) anisotropy of dielectric constant and strain within the $ab$ plane appears due to the orthorhombic distortion, and (3) the alignment of crystalline domains with applied magnetic field occurs, resulting in the large magnetic field dependence of dielectric constant and strain.

10:00AM X23.00011 Polar Behavior in a Magnetic Oxide Via A-Site Size Disorder. DAVID J. SINGH, ORNL, CHUL HONG PARK, Pusan National University — Density functional calculations are used to test a new mechanism for ferroelectricity in magnetic perovskites based on A-site size disorder. Calculations of the structure and magnetic ordering of (La,Lu)MnO$_3$ show that this mechanism is effective for this material, which is predicted to be both polar (ferroelectric or relaxor) and ferromagnetic, depending on the Lu concentration.

1 This work supported by DOE, DMS&E.
10:12AM X23.00012 Electric field control of magnetic phase transitions in Ni$_3$V$_2$O$_8$. P. KHAREL, C. SUDAKAR, Wayne State University, A.B. HARRIS, University of Pennsylvania, R. NAHK, G. LAWES, Wayne State University — In certain multiferroics, including Ni$_3$V$_2$O$_8$, the ferroelectric order is induced by the magnetic structure, leading to the simultaneous onset of spin and charge ordering. We have prepared thin films of Ni$_3$V$_2$O$_8$ by sputter deposition. Films annealed at 1000°C crystallize with closely packed rod-like grains. XRD confirms that the films are single phase Ni$_3$V$_2$O$_8$ and highly oriented along the b-axis. We observe a hysteretic magnetic anomaly at 3.6 K, which is consistent with a first order phase transition from a canted magnetic state to incommensurate magnetic order. This transition temperature is suppressed by $\Delta T$=0.2 K in an electric field of 30MV/m. An anomaly in the dielectric constant is observed at 6.3K, corresponding to a transition between two incommensurate magnetic states. Because the electric field acts as a field conjugate to the order parameter, it causes a rounding of the phase transition and an apparent increase in the transition temperature by $\Delta T$=0.2 K when the sample is biased at 25 MV/m. The E-T phase boundary for the 3.6 K phase transition is linear, while the 6.3 K phase boundary shifts roughly like E vs.$T^2$, consistent with estimates from critical scaling. We will discuss the electric field control of magnetic order parameter in these films and some important implications of this result for the multiferroic material thin film research.

10:24AM X23.00013 Direct Evidence of Magnetoelastic Coupling in Ni$_3$V$_2$O$_8$.1, LUCIANA I. VERGARA, J. CAO, J. L. MUSFELDT, University of Tennessee, N. ROGADO, R. CAVA, Princeton University, F. YEN, R. P. CHAUDHURY, B. LORENZ, University of Houston — We investigate the infrared active phonons of the Kagome staircase compound Ni$_3$V$_2$O$_8$ as a function of temperature to elucidate changes in magnetoelastic coupling through the cascade of low-temperature magnetic transitions. A detailed analysis of the a- and c-polarized vibrational mode trends demonstrates that: i) the approach to the cascade of magnetic transitions is driven by the high frequency stretching modes and the highest frequency bending mode along a; ii) the paramagnetic to high-temperature incommensurate phase transition is driven by low frequency c-polarized modes; and iii) the high-temperature to low-temperature incommensurate phase transition is driven by all a-polarized modes plus the NiO$_6$ stretching mode along c. Work is in progress to elucidate the trends along b. Overall, we find that the phonons are sensitive to the magnetic state, indicating that the lattice is flexible, coupling strongly to the spin system in this multiferroic material.

This work is supported by the U.S. Department of Energy.

10:36AM X23.00014 Magnetic field effect on the magnetic structure of Ba$_3$CoGe$_2$O$_7$. C.R. DELA CRUZ, S. LEE, Dept. of Physics and Astronomy, Univ. of Tennessee, Knoxville, S.-W. CHEONG, RCEM and Rutgers University, Picataway, N.J. Y. CHEN, J. LYNN, NIST-NCNR Gaithersberg, MD. H. MOOK, Neutron Scattering Science Division, ORNL, Oak Ridge, TN. P. DAI1, Dept. of Physics, Univ. of Tennessee — Multiferroic materials have recently attracted much interest fueled by the discovery of the coexistence and mutual interference of long range magnetic and ferroelectric order in them. Further attention to these compounds is gained due to their potential for device applications made possible by the controllability of the spontaneous polarizations by magnetic fields or the bulk magnetization by an electric field via the sizable magneto-dielectric coupling in them. The fundamental microscopic mechanism for the phenomena is yet to be fully understood but an essential component has been suggested to be the non-linear coupling of the ferroelectric and magnetic order parameters with a spatially varying magnetization. It is thus the focus of this work to study the static magnetic structure of the compound Ba$_3$CoGe$_2$O$_7$ below its magnetic and ferroelectric ordering temperature of 7K. Neutron diffraction measurements were done on the compound under applied magnetic fields up to 7 T along the crystal’s c-axis.

1also with the Neutron Scattering Science Division, ORNL.

Friday, March 14, 2008 8:00AM - 11:00AM
Session X24 DCMP: Nanotubes: Transport, Synthesis and Growth Morial Convention Center 216

8:00AM X24.00001 Quantum electron transport in toroidal carbon nanotubes. MARK JACK, MARIO ENCINOSA, Florida A&M University, Physics Department, Tallahassee, FL 32307. — Electron transport under bias is treated in tight-binding approximation using a non-equilibrium Green’s function approach. Density-of-states D(E), transmissivity T(E), and current I$_{CD}$ are calculated through a (3,3) armchair nanotorus with laterally attached metallic leads and a magnetic field penetrating the toroidal plane. Plateaus in T(E) through the torus are observed as a function of both the relative angle between leads and magnetic flux. Initial computational studies performed with 1800 atoms and attached leads show substantial computational slowdown when increasing the system size by a factor of two. Results are generated by inverting the device Hamiltonian with a standard recursion method extended to account for unit cell toroidal closure. Significant computational speed-up is expected for a parallelized code on a multiprocessor computer cluster. The dependence of electronic features on torus size and torus curvature is tested for three tori with 900, 1800 and 3600 carbon atoms, respectively. References: 1. M. Jack and M. Encinosa, Quantum electron transport in toroidal carbon nanotubes with metallic leads. ArXiv: quant-ph/0709.0760. 2. M. Encinosa and M. Jack, Dipole and solenoidal magnetic moments of electronic surface currents on toroidal nanostructures. J. Comp.-Aided Mat. Design (Springer), 14 (1) (2007) 65 – 71.

8:12AM X24.00002 Ab initio study of solvent effects on electrical transport of molecular bridge between electrodes. ARHIRO TAWARA, TOMOFUMI TADA, SATOSHI WATANABE, Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo and Creast, Japan Science and Technology Agency — The electrical conductance of benzene dithiolate (BDT) between gold electrodes has been actively investigated to realize single molecular devices. However, almost all of previous theoretical studies for the electrical conductance of BDT were done assuming 0K and vacuum in spite that many measurements have been performed at room temperature in solution [1,2]. In this study, we have investigated the electrical transport of BDT molecules in water solution using ab initio nonequilibrium Green’s function method and Car-Parrinello molecular dynamics at room temperature. The calculated time-averaged conductance of the BDT in water solution, 0.190 G$_0$, is clearly different from the value calculated without water, 0.201 G$_0$. Detailed analysis shows that this difference can be attributed to the effect of dipole moments of water molecules on the potential profile of the BDT molecule. [1] X. Xiao et al., Nano Lett. 4, 267 (2004). [2] M. Kiguchi et al., Appl. Phys. Lett. 89, 213104 (2006).

8:24AM X24.00003 Low-temperature electronic transport in Pt-nanocluster decorated alumina template grown carbon nanotubes. SWASTIK KAR, CATERINA SOLDANO, LI CHEN, Rensselaer Polytechnic Institute, SAIKAT TALAPATRA, University of Southern Illinois at Carbondale, ROBERT VAJTAI, SAROJ NAYAK, PULICKEL AJAYAN, Rensselaer Polytechnic Institute — Alumina template grown nanotubes are known to be highly disordered tube when compared to arc-discharge grown tubes. This is due to the particular type of growth process involved. Temperature dependence study reveals a slow power law dependence of the conductance as a function of the temperature. Large value of power law exponents found in pristine tubes, suggest that the transport mechanism takes place through tunneling between adjacent graphene flakes. When platinum-decorated, those devices show a Luttinger liquid behavior in the high-T regime and a large suppression of the conductance at low-T due to the interplay of disorder and e-e interactions. Transport properties are studied in light of a recently proposed model for disordered multi-channel quantum wires. Magneto-transport measurements (|B|<5T) show the presence of weak localization and a small but distinct Rashba spin-orbit scattering effect in the low-field regime (|B|<5T), the latter attributed to the surface decoration. Coherent transport is found to be recovered with increasing applied electric field.

8:36AM X24.00004 Electronic properties of doped semiconductor nanowires. MAMADOU DIARRA, CHRISTOPHE DELERUE, IEMN-ISEN, YANN-MICHEL NIQUET, CEA/DRFMC/SP2M/LSim, GUY ALLAN, IEMN-ISEN — Semiconductor nanowires have shown very promising properties, which opens new opportunities for the design of nanoscale devices. The physics of these nanowires is not yet fully understood. In this context, theory and numerical simulation give valuable insights. We present self-consistent tight binding calculations of donor and acceptor impurities in semiconductor nanowires, either in a free standing configuration or surrounded by a metallic gate and an oxide. We show that the dielectric mismatch between the nanowires and their surroundings increases the binding energies of dopant impurities up to a few hundreds of meV [1]. This decreases the doping efficiency and affects the behavior of nanowire devices. The effect of the environment will be discussed. When the nanowires are surrounded by an oxide, polaronic effects largely contribute to the binding energy of the dopants [2].


8:48AM X24.00005 The effect of the sodium and iodine doping on the electronic band structure of the polyicosahedral Si nanowire: A first principles study. KENGO NISHIO, Research Institute for Computational Sciences (RICS), National Institute of Advanced Industrial Science & Technology (AIST), TAIŞŬKE OZAKI, TETSUYA MORISHITA, WATARU SHINODA, MASUHIRO MIKAMI, JAIST — In a previous molecular dynamics study, we predicted a polyicosahedral Si nanowire which has a Si20 fullerene cage per icosahedral Si100 nanodot [1]. The unique cage structure is distinct from the crystalline diamond Si nanowire. Encapsulating a guest atom into the Si20 cage allows us to tune the physical properties of the nanowire. Here, we report on a first-principles study of the effect of the sodium and iodine doping on the electronic band structure of the hydrogen-terminated polyicosahedral Si nanowire [2]. Our calculations reveal that the guest-free polyicosahedral Si nanowire is a semiconductor with a 1.20 eV band gap. We also find that the semiconducting nanowire becomes metallic by the sodium and iodine doping, suggesting that the electronic band structure of polyicosahedral Si nanowires can be tuned by doping appropriate guest atoms. [1] J. Chem. Phys. 125, 074712 (2006). [2] submitted to PRB

9:00AM X24.00006 Electronic structures and electron-phonon interactions of boron-doped carbon nanotube. TAKASHI KORETSUNE, SUSUMU SAITO, Tokyo Institute of Technology — We study the boron-doped single-walled carbon nanotubes using first-principles method based on the density functional theory. The total energy, band structure and density of states are calculated. From the formation energy of boron-doped nanotubes with different diameter, it is found that the narrower tube needs lower energy to substitute a carbon atom with a boron atom. Using the result of different doping rate in the (10,0) tube, we extrapolate the result to low boron density limit and find that the ionization energy of the acceptor impurity level is approximately 0.2 eV. Furthermore, we discuss the doping rate dependence of the density of states at the Fermi level and the electron-phonon interactions which are important for superconductivity.

9:12AM X24.00007 Edge states and magnetism in carbon nanotubes with line defects. HELIO CHACHAM, MARIO S. C. MAZZONI, SIMONE S. ALEXANDRE, Universidade Federal de Minas Gerais — Under certain conditions, magnetic ordering has been predicted to occur in carbon nanostructures even in the absence of transition metal impurities. These conditions involve situations in which electronic localization takes place, such as at zig-zag edges or defects in graphene sheets and ribbons or in topological defects in carbon nanostructures. In the present work, we apply first-principles calculations to investigate the interplay between electronic and magnetic properties of carbon nanotubes with line defects. We consider three types of defects: lines of C-O-C epoxy groups, and defects resulting from the substitution of the oxygen atoms by CH2 or C2H4 divalent radicals. We find that the line defects behave as pairs of coupled graphene edge states, and a variety of electronic and magnetic ground states is predicted as a function of defect type, nanotube diameter, and a possibly applied transverse electric field.

9:24AM X24.00008 Effects of intrinsic spin-orbit coupling in carbon nanotubes1. CARLOS A. BÜSSE, MAHDI ZAREA, NANCY Sandler, Department of Physics and Astronomy, Ohio University, Athens OH 45701 USA. — The electronic structure and transport properties of carbon nanotubes (NTs) are the subject of intense theoretical and experimental studies. Tight-binding model predict these quasi-1D systems to be metallic or insulating depending on their chiral wrapping. Furthermore, external magnetic fields applied along the NT’s axis, are expected to change these behaviors by opening (metallic) or closing (insulating) gaps. In this work we present preliminary numerical results obtained solving a tight-binding Hamiltonian [1] for band structures of armchair and zigzag NTs in the presence of the intrinsic spin-orbit (I-SO) interaction and magnetic fields. The I-SO interaction has dramatic effects, opening gaps for metallic NTs that are proportional the I-SO coupling constant. When considering an external field, the I-SO generated gaps show a quadratic dependence on the field strength in contrast with the linear dependence predicted in the absence of this interaction. Insulating tubes show increased gaps that do not close even in the presence of external fields.


9:36AM X24.00009 Transport properties of single vacancies in nanotubes. ALEXANDRE R. ROCHA, J.E. PADILHA, ADALBERTO FAZZIO, ANTONIO J.R. DA SILVA, Instituto de Física - USP Brazil — We present transport, density of states and electronic transport calculations of single vacancies in carbon nanotubes. We confirm that the defect reconstructs into a pentagon and a nonagon following the removal of a single carbon atom. This leads to the formation of a dangling bond. Finally we demonstrate that care must be taken when calculating the density of states of impurities in one dimensional systems in general. We show that obtaining information about the transport properties of such systems with defects solely from the density of states of a periodic DFT calculation can be misleading. The appearance of mini-gaps and oscillations, even in the limit of large unit cells, can be erroneously associated with changes induced by the defect itself instead of a figment of the procedure. In fact, we demonstrate that those mini-gaps vanish if the appropriate approach is taken, namely a Green’s function method where the effects of semi-infinite electrodes are considered and a true open system is calculated.

9:48AM X24.00010 The structural and electronic properties of vacancy clusters in carbon nanotubes. ALEX TAEKYUNG LEE, YONG-JU KANG, KEE JOO CHANG, Korea Advanced Institute of Science and Technology — Carbon vacancies, which can be generated by electron or ion irradiation, significantly modify the structural and electronic properties of carbon nanotubes. Recent experiments showed that vacancy-type defects induce structural changes such as junction, shrinkage, and bending. In this work we study the atomic and electronic structure of vacancy clusters up to six missing atoms in carbon nanotubes through both first-principles and tight-binding calculations. We find that vacancy defects are generally stable when they are aligned along the tube axis, forming a vacancy-chain. Due to the curvature effect, this feature is different from that found for graphene, where vacancies tend to aggregate into a lump. For the even-numbered vacancies in the (5,5) and (9,0) nanotubes, we find that clustering of vacancies leads to the local shrinkage, with a smaller diameter tube sandwiched between two semi-infinite tubes. In this case, the defect levels near the Fermi level are mostly associated with 7- or 8-membered rings, whereas those for odd-numbered vacancies result from the remnant dangling bonds.
10:00AM X24.00011 Synthesis of Triangle Tungsten Oxide Nanosheets with Potassium Doped - RONG HU, KUNQUAN HONG, HUASHENG WU — We report that large quantity of tungsten oxide nanosheets are synthesized by oxidizing tungsten plate directly. Using potassium hydrate as the catalyst and tungsten plate as the substrate, those triangle tungsten oxide nanosheets with thickness of 50-300 nm and wide up to tens of micrometers are obtained on a large scale. The angles of the triangle nanosheets are around 35° and 50° statistically. We discussed the potential reason of this peculiar phenomenon, besides the several characterizations results of the grown nanosheets. The probable growth mechanism is also investigated.

10:12AM X24.00012 CVD synthesis of graphene — TAO JIANG, JOEL THERRIEN, U. Massachusetts-Lowell — We will report on the use of Chemical Vapor Deposition (CVD) to grow sheets of graphene on substrates suitable for the semiconductor industry. Growth starts with the deposition of seed crystals of graphene on the substrate. CVD growth is found to result in growth at the edges of the seeds, rather than on the surfaces. The result is increases in the size of the seed crystal without additional layers of graphene forming on top of the crystal. This technique holds promise for forming large areas of high quality single layer graphene on inexpensive substrates.

10:24AM X24.00013 New opportunities from controlled growth of carbon nanotubes — SEOKWOO JEON, ROBERT CALDWELL, YUYAO SHAN, HANFEI WANG, JINYAO TANG, SAMI ROSENBLATT, COLIN NUCKOLLS, JAMES HONE, Columbia University — Aligned growth of carbon nanotubes (CNT) has been an important issue to researchers involved in CNT, and recent work has proved the possibility of alignment by using special substrates (i.e. quartz, sapphire, etc.) where CNT can grow along crystallographic axes. We present here two applications of aligned tubes produced from quartz substrates. The first is the realization of an integrated platform for using CNTs as electrodes for single molecules toward sensing applications; numerous sensing units can be generated by photolithography without long, tedious e-beam writing steps due to the precise control of location and direction of CNTs over a large area (~1X1 cm). The second is measurement of the high frequency properties of CNTs, which is difficult due to the high impedance of single-tube devices. By a slight modification of growth parameters, we have achieved growth of ‘serpentine’ CNTs on quartz substrates that permit the fabrication of low-impedance devices using multiple identical CNT sections.

10:36AM X24.00014 Diffusion-limited and pressure-driven electrodeposition in a microfluidic channel — GEOFF STEEVES, University of Victoria, ALEX WLASENKO, DENNIS ZAKOPCAN, DAVID SINTON, University of Victoria — Self-terminating electrochemical fabrication has previously been devised to create quantum point contacts with single-atom contacts, but the structure of the growth has been poorly controlled. We have introduced a microfluidic channel with which to apply pressure-driven flow during the formation of the junction between two Au electrodes. Without applied flow, dendritic growth and dense branching morphologies were typically observed at the cathode. The addition of applied pressure-driven flow resulted in a densely packed gold structure that filled the channel. Our computer simulation yielded insight into the regimes where the diffusion, flow and electric field between the electrodes individually dominated growth. Proposals for further sophistication in both experiment and simulation will also be presented.

1This project is supported by CFI, BCKDF, NSERC and CAMTEC.

10:48AM X24.00015 Continuous and Scalable Fabrication of Transparent Conducting Thin Films of Single Walled Carbon Nanotubes — BUDHAPADA DAN, MAINAK MAJUMDAR, MATTEO PASQUALI, Rice University — We report the fabrication of optically transparent and electrically conducting thin films of single-walled carbon nanotubes (SWNT) using the industrially scalable, fast and simple process of Rod-Coating. Rheology was used to study four different surfactants, their capacity to disperse SWNT in water and the viscoelastic properties of the resulting dispersion. A combination of two different surfactants was found ideal to make a uniform dispersion with high concentration of SWNT and the specific viscoelastic properties desired for coating. Rod coating with this coating fluid produced highly uniform, transparent and conducting SWNT thin films. The films were also treated with various strong acids which lead to further significant improvement in properties. Our results show that the choice of surfactant for making the coating dispersion has a strong effect on the electro-optical properties of the SWNT films. Films with sheet resistance of 100 Ohm/sq and 300 Ohm/sq for respective transparency of 70% and 90%, in the visible region, were obtained with this process. The development of this continuous and scalable fabrication process will thus bring the SWNT films closer to commercial application.

Friday, March 14, 2008 8:00AM - 11:00AM — Session X25 DPOLY: Block Copolymer Phase Behavior Morial Convention Center 217

8:00AM X25.00001 Molecular Simulation of Bicontinuous Phases in Diblock Copolymer Melts — FRANCISCO MARTINEZ-VERACOECHEA, FERNANDO ESCOBEDO, Cornell University — Molecular simulations are used to study the stabilization of different bicontinuous phases in diblock copolymer (DBC) melts. The stabilization approach entails attempting to reduce the packing frustration inside the bicontinuous phases nodes by the addition of a ‘filler’ with affinity for the A component. Two different strategies are considered: 1) addition of selective- solvent particles, and 2) addition of homopolymer. Approximate phase boundaries were found via free-energy calculations. A very dissimilar phase behavior is observed upon increasing the amount of the “additive” in the two different strategies. While with the first strategy (i.e., addition of selective solvent) we observed the progression Gyroid (G) → Perforated Lamellae (P) → Lamella → Reversed-Gyroid. With the second strategy (i.e., addition of homopolymer) we observed the progression of morphologies G → Cylinder → Double Diamond (DD) → Plumber’s Nightmare (P). In both the DD and the P phases, the homopolymer concentrates preferentially in the nodes, suggesting the reduction of the nodes’ packing frustration. In addition, a novel morphology was observed, wherein cylinders of two different diameters alternate in a tetragonal packing. The contrasting difference in the phase behavior observed for the two strategies is understood as a consequence of the difference in mixing entropy exhibited by the two additives.

8:12AM X25.00002 Orthonormhic Fddd Network in Diblock Copolymer Melts — MIKIHITO TAKE-NAKA, MYUNG IM KIM, SATOSHI AKASAKA, TSUTOMU WAKADA, SHOTARO NISHITSUJI, HIROKAZU HASEGAWA, Kyoto University — Poly(styrene-block-polyisoprene) (S-I) diblock copolymer melts with asymmetric volume fraction are shown to form an orthonormhic Fddd network structure, which Tyler et al. predicted with self-consistent field theory for diblock copolymer melts. The studies with small-angle X-ray scattering and transmission electron microscopy revealed that the microphase-separated structure of the S-I diblock copolymer melts with asymmetric volume fraction shows the sequence of transition of disorder-ordered phase with decreasing temperature. Fddd phase appears within the narrow composition and temperature range where gyroid, lamella, and hexagonally perforated layer (HPL) phases appear. The ratio of unit cell parameters (a:b:c) estimated from the peak positions of the scattering function is 1:2:00:3.51, which agrees with the result of the theoretical calculation by Tyler et al. In this orthonormhic structure with the observed unit cell parameters, the higher order reflections 022, and 004 overlaps with the reflection 111 at the first order peak.

1This research is partially supported by Japan Society for the Promotion of Science, Grant-in-Aid for Scientific Research(C), 19550206, and Grant-in-Aid for Scientific Research(S), 17105004.
8:24AM X25.00003 Fluctuation effects in block copolymers, ERIN M. LENNON, RICHARD ELLIOTT, GLENN H. FREDRICKSON, University of California, Santa Barbara — Using recently developed techniques for locating phase transitions, we study the effects of fluctuations in a field theoretic model on block copolymer behavior. Specifically, we couple the use of complex Langevin dynamics within a field theoretic framework and thermodynamic integration techniques for the calculation of free energies of fluctuating systems to show a revised prediction of the diblock copolymer phase diagram. Further, these methods are extended into blend systems to investigate unbinding transitions and critical micelle concentrations in cylindrical phases.

8:36AM X25.00004 Scaling of Diblock Copolymer Lamella near the Order Disorder Transition, ANDREW B. CROLL, AN-CHANG SHI, KARI DALNOKI-VERESS, McMaster University — Our accumulated knowledge of the physics of diblock copolymer phase transitions is extensive after decades of intense interest. There are, however, several inconsistencies between experiment and current theoretical understanding. Nanosamples are prepared from block copolymer solutions using high aspect ratio nanohole template holders. By significantly out of agreement with theory near the order disorder transition (ODT), this length scales as $(\chi N)^m$ where $\chi$ is the Flory–Huggins interaction parameter and $N$ is the number of monomers. Experiments yield $m = 0.8$ while theory predicts $m = 1$. We use optical microscopy to make real space measurements of the thickness of symmetric polystyrene - block - poly (2 vinyl pyridine), which we find to scale linearly - as predicted by theory. Our experiment suggests two simple optical methods for the measurement of $\chi$.

8:48AM X25.00005 Self-assembly of Asymmetric Architectures: Study of the Phase Behavior of an ABAC Block Copolymer, MICHAEL BLUEMLE, GUILLAUME FLEURY, TIMOTHY LODGE, FRANK BATES, University of Minnesota, Department of Chemical Engineering and Materials Science — We have investigated the bulk phase behavior of the asymmetric tetra-block poly(cyclohexylethylene-b-ethylene-b-cyclohexyethylene-b-dimethylsiloxane) (CECD) in order to elucidate the effects of asymmetry created by introducing a third chemically distinct block to the well-studied CEC triblock. These tetra-block polymers are especially attractive due to the potential of degrading the D block, leaving a mechanically robust polyoldefin nanoprotransport material. Starting with CEC triblocks that self-assemble into different morphologies (hexagonally packed cylinders and lamellae), varying amounts of D have been added, creating two series of polymers along distinct isothetics. A combination of small-angle x-ray scattering, transmission electron microscopy and dynamic mechanical spectroscopy have revealed the complex phase behavior of these asymmetric polymers. Addition of as little as nine percent D by volume drastically changes the tetra-block morphological behavior as compared to their precursor CEC triblocks. These promising results exhibit the influence of asymmetry on the self-assembly of complex architectures in block copolymers.

9:00AM X25.00006 Soft and Strong Thermoplastic Elastomers Through Molecular Design, FOLUSHO OYEROKUN, GLENN FREDRICKSON, UCSB, DALE HANDLIN, Kraton Polymers — Thermoplastic elastomers (TPE) that have a low linear modulus and yet are strong at large extension are of great importance in a variety of technological applications. Current TPE designs based on ABA triblock copolymers are limited in that the maximum volume fraction of the hard A blocks, which correlates with the material strength, is restricted by the constraint that the A domains be discrete while the soft B domains are continuous. In this study, we have investigated new designs of TPEs that utilize polydispersity of the hard blocks in tandem with novel block architectures to control morphology in microphase separated AB block copolymers. Self-consistent field theory calculations confirm that these designs stabilize spherical and cylindrical phases at higher volume fractions of the hard blocks, with the maximum volume fraction of the hard block in some cases approaching twice that of a conventional ABA thermoplastic elastomer.

9:12AM X25.00007 Influence of Soft Segment Composition on Phase Separated Microstructure of PDMS-Based Multiblock Polyurethane Copolymers, TAEYI CHOI, Penn State University, JADWIGA WEKSLER, AJAY PADALGIKAR, AorTech Biomaterials, JAMES RUNT, Penn State University — Multiblock polyurethane (PU) copolymers with polydimethylsiloxane (PDMS) based soft segments possess intriguing microphase separation behavior and excellent biocompatibility. In this study we investigate the microphase-separated structure of PDMS-PUs with various well-defined soft segment compositions, which is closely connected to the structural and surface properties of these copolymers. The PDMS-PUs are shown to exhibit a three phase, core-shell like morphology. Intra- and intercomponent hydrogen bonding was explored using FTIR spectroscopy and quantitative analysis of hard/soft segment mixing was determined by small-angle X-ray scattering. The presentation will focus on the latest findings, particularly the role of PDMS in controlling the details of the microphase-separated texture.

9:24AM X25.00008 Nanoparticle-Regulated Phase Behavior and Morphological Development in an Ordered Block Copolymer, MICHELLE BOWMAN, North Carolina State University, STEVEN SMITH, Procter & Gamble Co., JON SAMSETH, SINTEF Materials & Chemistry, MICHAEL BOCKSTALLER, Carnegie Mellon University, RUSSELL THOMPSON, University of Waterloo, KIM RASMUSSEN, Los Alamos National Laboratory, RICHARD SPONTAK, North Carolina State University — Although microphase-ordered block copolymer motifs are employed to template inorganic nanoparticles, only recently has the effect of nanoparticles on copolymer self-assembly been explored. In this work, we examine the influence of nanoparticles on the copolymer order-disorder transition (ODT) temperature. Theoretical results from a hybrid self-consistent field/density functional theory — supported by experimental observations of a model copolymer/nanoparticle system — confirm that judicious selection of nanoparticle size and selectivity can be used to increase the ODT temperature at constant concentration. For a given nanoparticle size and selectivity, we show that there likewise exists a critical nanoparticle concentration beyond which the ODT temperature decreases. The ability of nanoparticles to increase the ODT temperature is a unique consequence of their size and is not expected for small-molecule additives. At high concentrations, the nanoparticles form percolated colloidal networks that represent highly confined environments for the copolymer molecules.

9:36AM X25.00009 Effects of Lithium Salts on the Domain Size of Polyethylene Oxide Containing Block Copolymers, NISITA WANAKULE, SCOTT MULLIN, NITASH BALSARA, UC Berkeley — The morphology of block copolymers with and without lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salts are measured with small-angle x-ray scattering (SAXS). The block copolymers comprise of polyethylene oxide (PEO), a polymer with a higher dielectric constant that dissolves LiTFSI, and polystyrene (PS), a polymer with a lower dielectric constant that does not dissolve LiTFSI. Due to the hygroscopic nature of the salts, blend preparation is performed completely in a glovebox and the SAXS samples are sealed off in airtight sample holders. To ensure that moisture contamination does not affect morphology, Karl-Fischer titrations are performed after SAXS measurements. Our data will be compared with literature results that indicate a 300% increase in the domain spacing of PEO-containing block copolymers spacing due to the addition of LiTFSI.

9:48AM X25.00010 Weak Segregation Theory of Microphase Separation in Block Copolymers: New Results and Perspectives, IGOR ERUKHIMOVICH, Moscow State University — The weak segregation theory (WST) of microphase separation in block copolymers (BC) is based on the vision by Landau (1937) and seminal breakthrough by Leibler (1980) into microscopic theory of as well as the Brazovskii-Fredrickson-Helfand (1975, 1987) understanding of the corresponding fluctuation effects. The WST is especially helpful in the situation when the ODT temperature decreases. The ability of nanoparticles to increase the ODT temperature is a unique consequence of their size and is not expected for small-molecule additives. At high concentrations, the nanoparticles form percolated colloidal networks that represent highly confined environments for the copolymer molecules.
10:00AM X25.00011 Tunable Microphase Segregation of Gradient Copolymers: Ordering in Materials with Sinusoidal Composition Profiles, MICHELLE MOK, WESLEY BURGHARDT, JOHN TORKELSON, Northwestern University — Gradient copolymers are a class of polymers that exhibit a gradual change in composition along the entire chain from mostly A-monomer to mostly B-monomer. Theoretical work has predicted that gradient copolymers organize into sinusoidal composition profiles rather than the step-like profiles seen for block copolymers. Here, small-angle x-ray scattering and rheological studies were performed to investigate the impact of gradient design and comonomer choice on this unique ordering. Samples showed a variety of non-terminal behaviors consistent with their chain architecture relative to block copolymers, indicating highly tunable microphase segregation. Scattering results also demonstrated that a range of ordering is attained, with higher order peaks visible in more microphase-segregated samples. In addition, it was demonstrated for the first time that application of high amplitude oscillatory shear induced domain shear alignment in a manner similar to block copolymers, even though gradient copolymers do not possess distinct domain boundaries.

10:12AM X25.00012 Polydispersity effects in block copolymer melts1, MARK MATSEN, Department of Mathematics, University of Reading — We examine the effects of polydispersity on the phase behavior of diblock copolymer melts using self-consistent field theory (SCFT). The calculations are performed with an efficient spectral-based algorithm that can handle high degrees of polydispersity with only a modest increase (i.e., a factor of 2 or 3) in computational cost over that of monodisperse melts [Matson, EPJE, 21, 199 (2006)]. We find that even small degrees of polydispersity can have a significant effect on the domain sizes and the position of the phase boundaries. For large polydispersities, fractionation also becomes important and the phase diagram develops large two-phase coexistence regions [Matson, PRL, 99, 148304 (2007)]. As a consequence, the complex gyroid phase becomes unstable with respect to the coexistence of lamellae and cylinders.

1This work was supported by EPSRC (EP/E010342)

10:24AM X25.00013 Polydispersity-Driven Morphological Transitions in ABC Triblock Terpolymers, ADAM J. MEULER, CHRISTOPHER J. ELLISON, CHRISTOPHER M. EVANS, University of Minnesota Department of Chemical Engineering and Materials Science, MARC A. HILLYER, University of Minnesota Department of Chemistry, FRANK S. BATES, University of Minnesota Department of Chemical Engineering and Materials Science — The use of synthetic polymerization techniques (e.g., controlled radical polymerizations) that often yield polydispersity indices greater than 1.1 is becoming more widespread. Advances in these methodologies have increased the number of monomers amenable to incorporation in block copolymers and will potentially drive commercial costs down. Since many block copolymer properties are governed by the underlying mesostructure, understanding the influence of polydispersity on morphological behavior should prove vital to the success of block copolymer commercialization efforts. This presentation will focus on polydispersity-driven morphological transitions in poly(isoprene-b-styrene-b-ethylene oxide) (ISO) triblock terpolymers. ISO triblocks with polydisperse polystyrene blocks were prepared by anionic polymerization and their morphological behavior was characterized using small-angle x-ray scattering and dynamic mechanical spectroscopy. Only lamellar microstructures were identified along the f1 = f2 isopleth for polydisperse ISO triblocks, while an orthorhombic network (O(3)) was previously identified in monodisperse ISO triblocks.

10:36AM X25.00014 Scaling of the ODT of Block Copolymers in Compressed CO2, CURRAN CHANDLER, TIMOTHY FRANCIS, JAMES WATKINS, University of Massachusetts, Amherst; Department of Polymer Science & Engineering — It is well-known that diblock copolymers with sufficient χN form periodic microphase-separated domains upon cooling through an order-disorder transition (ODT). We have investigated the scaling behavior of the ODT as a function of polymer volume fraction, ϕ, of several nearly symmetric poly(styrene-2-vinylpyridine) and poly(styrene-isopropene) diblock copolymer/diluent systems in relation to the well-known dilution approximation. Using compressed CO2 in the place of conventional liquid diluents allowed the determination of the scaling parameter, α, for highly concentrated systems where ϕ ranges from 0.85 to 1.0 at high temperatures. The scaling was determined by combining optical birefringence measurements of the ODT (λODT) with the ellipsometric swelling measurements (α) of the constituent homopolymers at increasing CO2 pressures. We show that sorption of small volume fractions of CO2 results in significant reductions in the observed ODTs. Yet, α was clearly shown not to be universal even for a specific diblock copolymer. For styrene-isopropene copolymers, it appears that α is an increasing function of copolymer molecular weight, with α taking on both positive and negative values.

1Currently at BASF

10:48AM X25.00015 Pressure Effect on Phase Behavior of Weakly Interacting Block Copolymers by using FTIR spectroscopy, HYE JEONG KIM, SEUNG BIN KIM, JIN KON KIM, Pohang Univ. of Sci. Tech., YOUNG MEE JUNG, Kangwon National University, YOUNG MEE JEONG COLLABORATION — Hydrostatic pressure effect on the phase transition of polystyrene-block-poly(n-pentyl methacrylate) [PS-b-PnPMA] copolymer was investigated by FTIR spectroscopy. The size of closed-loop consisting of both the lower disordered-to-ordered transition and the upper ordered-to-disordered transition became smaller with increasing pressure. The functional groups belonging to the PS block are much more sensitive to pressure compared with those belonging to the PS block. The sensitivity of the functional groups change with pressure is different from that with temperature.

1This work was supported by Creative Research Initiative Program supported by KOSEF

Friday, March 14, 2008 8:00AM - 11:00AM –
Session X27 GMAG: Focus Session: Exchange Bias and Magnetic Interactions Morial Convention Center 219

8:00AM X27.00001 Uncompensated moments in antiferromagnets: Origin and role in exchange bias, IGOR V. ROSCHCHIN, Physics Department, University of California, San Diego and Texas A&M University, ZHI-PAN LI, Physics Department, University of California, San Diego and University of South Florida, MARIA VARELA, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory, IVAN K. SCHULLER, Physics Department, University of California, San Diego — Exchange bias (EB) is a ferromagnet (FM) – antiferromagnet (AF) proximity effect. The depth profile of the magnetization across the interface between a FM (Co) and an AF (FeF2) in an EB system has been measured. [1] It was found that both uncompensated and compensated magnetic moments are present in FeF2. The origin of these moments remains an open question. Our high-resolution STEM study confirms that FeF2 grows epitaxially on MgF2, and its structural quality is very high. It also reveals that the substrate surface imperfections do not necessarily affect the quality of the FeF2 layer. In magnetization measurements of just a thin film of FeF2, without a FM, we find an uncompensated magnetization. This magnetization demonstrates temperature dependence and horizontal hysteresis loop shift, typical for EB. Dependence of this magnetization on the substrate, film parameters and cooling conditions will be discussed. Work supported by US DOE.

8:12AM X27.00002 Strong anisotropy suppression at the CoO Neél temperature in perpendicularly exchange-biased CoO/CoPt multilayers. ERIK SHIPTON, KEITH CHAN, UC San Diego, OLAV HELLWIG, Hitachi GST, ERIC E. FULLERTON, UC San Diego — We have performed high-field torque magnetometry measurements on perpendicularly exchange-biased CoO/CoPt multilayers. From magnetometry measurements we observe perpendicular exchange bias that goes to zero at a blocking temperature of 200 K. Torque measurements were performed from 2 to 400 K in fields up to 9 T. There is significant hysteresis even at 9 T fields suggesting instabilities in the AF layer. This hysteresis persists up to the blocking temperature. Surprisingly, there is a large reduction in the uniaxial anisotropy with increasing temperature with a minimum at 250 K, the estimated Neél temperature of the CoO layers, followed by an increase in the anisotropy with increasing temperature. The anisotropy of Co/Pt multilayers without the CoO layers monotonically decreases with increasing temperature. This suggests that there is an additional planar anisotropy arising from the CoO that counters the anisotropy of the Co/Pt layers, and that the contribution from the CoO is maximized at the Neél temperature as observed by Grimsditch et al. [1]. These results show that the addition of antiferromagnetic layers may be used to tune the temperature dependence anisotropy response of magnetic systems. [1] M. Grimsditch et al., Phys. Rev. Lett. 90, 257201 (2003).

8:24AM X27.00003 Pinned magnetization in the exchange bias system Permalloy/CoO. SUJOY ROY, Advanced Light Source, Lawrence Berkeley National Laboratory, ELIZABETH BLACKBURN, University of California, San Diego, CECILIA SANCHEZ-HANKE, Brookhaven National Laboratory, SUNIL SINHA, AMI BÉKOWITZ, University of California, San Diego — Interfacial effects are understood to be crucial in the development of exchange bias. In particular, the role of uncompensated spins is important, although because the interface is buried these uncompensated spins can be difficult to measure. Penetrating radiation such as neutrons or x-rays are one of the few tools available to do this. The problem of exchange bias is further complicated by the myriad differences observed from system to system, indicating that the local environment of the magnetic ions has a strong effect on the type of coupling that dominates across the interface. In turn, understanding this coupling is vital in understanding the microscopic origin of exchange bias in a given system. In this paper, we present soft x-ray reflectivity data that show that in the exchange biased state (i.e. below the Neél temperature 289 K for CoO) there is an interfacial layer between the Py and CoO that possesses a net magnetization at room temperature. In the exchange biased state, this contains the uncompensated spins from the CoO layer, and a significant fraction of the spins in this layer are pinned.

8:36AM X27.00004 Ultrafast frustration in the magnetization in exchange biased Ni/FeF$_2$. AMIT PORAT, School of Physics and Astronomy, Tel-Aviv University, Tel Aviv 69978, Israel, IVAN K. SCHULLER, Physics Department, University of California - San Diego, La Jolla, CA 92093-0319, SHIMSHON BAR-AD, School of Physics and Astronomy, Tel-Aviv University, Tel Aviv 69978, Israel — We used the magneto optical Kerr effect to study fast optically-induced magnetization dynamics in a Ni/FeF$_2$ exchange bias bilayer. We find that sub-picosecond laser pulses trigger an unexpected out of plane precession of the Ni magnetization, surprisingly in external magnetic fields that overcome the exchange bias (unlike previously reported precessions in bilayers). Even more surprisingly the precession persists for excitation intensities that completely decouple the Ni from the FeF$_2$. The experimental results suggest that the FeF$_2$ layer even at the thermally-excited interface is frustrated by the opposing antiferromagnetic fields created by the external field, the Ni layer, and the underlying thermally unexcited FeF$_2$ layer. The frustrated FeF$_2$ layer reorients, which in turn triggers the precession of the Ni. This implies that the decoupling at high excitation intensities does not only involve the Ni, but also the interfacial FeF$_2$ layer, which decouples from the cold underlying bulk FeF$_2$. The decoupling thus leads to a reversal of the exchange bias, as we found experimentally.

1Work supported by ISF grant 850/05 and the US-DOE.

8:48AM X27.00005 Antiferromagnetic Domain Size Measurement in Fe$_{0.70}$Zn$_{0.30}$F$_2$/Co Bilayers. DAVID LEDERMAN, HONGTAO SHI, Dept of Physics, West Virginia University, MICHAEL FITZSIMMONS, Los Alamos National Laboratory — The size of the antiferromagnetic domains of an epitaxial (110) Fe$_{0.70}$Zn$_{0.30}$F$_2$ doped layer is measured by ferromagnetic resonance. The antiferromagnetic Fe$_{0.70}$Zn$_{0.30}$F$_2$ layer is significantly narrower at the switching temperature than at either 25 or 30 K. This result is consistent with models that predict an inverse relationship between the antiferromagnetic domain size and exchange bias.

1Supported by the National Science Foundation at WVU (grant DMR-0400578) and the Dept of Energy at LANSCE.
2Presently at Dept of Physics, Sonoma State University

9:00AM X27.00006 Scaling behavior of the exchange-bias training effect. SRINIVAS POLISETTY, SARBESWAR SAHOO, CHRISTIAN BINEK, University of Nebraska-Lincoln — The dependence of the exchange-bias training effect on temperature and ferromagnetic film thickness is studied in detail and scaling behavior of the data is presented. Thickness-dependent exchange bias and its training are measured using the magneto-optical Kerr effect. A focused laser beam is scanned across a Co wedge probing local hysteresis loops of the Co film which is pinned by an antiferromagnetic CoO layer of uniform thickness. A phenomenological theory is best fitted to the exchange-bias training data resembling the evolution of the exchange-bias field on subsequently cycled hysteresis loops. Best fits are done for various temperatures and Co thicknesses. Data collapse on respective master curves is achieved for the thickness and temperature-dependent fitting parameters as well as the exchange bias and coercive fields of the initial hysteresis loops. The scaling behavior is strong evidence for the validity and the universality of the underlying theoretical approach based on triggered relaxation of the pinning layer towards quasi-equilibrium. [1] Srinivas Polisetty, Sarbeswar Sahoo, Christian Binek, Phys. Rev. B 76, 184423 (2007).

2This work is supported by NSF through career Grant No. DMR-0547887, the Nebraska Research Initiative (NRI), and by the MRSEC Program of the NSF (Grant No. DMR-0213808).

9:12AM X27.00007 Interlayer coupling in Co/NiO/Fe trilayers studied by element-specific XMCD and XMCD effects. J. WU, J. CHOI, Dept. of Physics, Univ. of California at Berkeley, Berkeley, CA 94720, C. WON, Dept. of Physics, Kyung Hee Univ., Seoul 130-701, Korea, A. SCHOLL, A. DORAN, E. ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, Y.Z. WU, X.F. JIN, Dept. of Physics, Fudan Univ., Shanghai 200433, P. R. China, Z.Q. QIU, Dept. of Physics, Univ. of California at Berkeley, Berkeley, CA 94720 — Co/NiO/Fe layers are grown on Ag(001) substrate using Molecular Beam Epitaxy (MBE). Element-specific magnetic domain images on both ferromagnetic (FM) Co and Fe layers and antiferromagnetic NiO layer are obtained using X-ray Magnetic Circular Dichroism (XMCD) and X-ray Linear Dichroism (XMLD), respectively. By comparing these magnetic domain images, we find that the Co-Fe interlayer coupling across the NiO spacer layer exhibits a transition from a 90°-coupling to a collinear coupling as the NiO film thickness increases. This observation is shown to be directly related to the NiO magnetic structure and its interaction at the Co/NiO and NiO/Fe interfaces.
9:24AM X27.00008 Thermodynamics of Co/Cr superlattices1, T. MUKHERJEE, S. SAHOO, R. SKOMSKI, D.J. SELLMYER, CH. BINEK, University of Nebraska-Lincoln — Progress in ultra thin film growth has resulted in many novel surface and interface induced properties of artificial heterostructures. Here, we study magnetic superlattices of ultrathin Co and Cr films grown by Molecular Beam Epitaxy methodology at a base pressure below 1×10^{-10} mbar. Our approach is based on controlling two distinct magnetic degrees of freedom. First, the critical temperature, T_c, of individual Co films is tailored via geometrical confinement of the correlation length perpendicular to the film. Various thickness dependent values, T_c, between zero and the bulk Curie temperature of 1388 K are realized. Second, the T_c-tailored Co films are antiferromagnetically coupled through Cr interlayer films. The oscillating coupling strength is tailored via the Cr interlayer thickness. The resulting thermodynamic properties of such Co/Cr superlattices are studied with the help of SQUID magnetometry. Particular emphasis is laid on tailoring magnetic entropy changes in the vicinity of room temperature. X-ray diffraction and X-ray reflectivity are used to correlate structural data with the magnetic properties.

1Financial support by Nebraska Center for Energy Sciences Research (NCESR) and NRI is gratefully acknowledged.

9:36AM X27.00009 Cooling Field Dependence of Magnetization Depth Profiles in Exchange-coupled Superlattices1, MICHAEL FITZSIMMONS, Los Alamos National Laboratory, KARINE DUMESNIL, CATHERINE DUFOUR, Laboratoire de Physique des Matériaux, Université Henri Poincare Nancy, France — In DyFe2/YFe2 superlattices, competition between ferromagnetic exchange coupling of adjacent Fe spins and antiferromagnetic coupling of Fe spins with rare earth spins leads to an antiparallel arrangement (confirmed with XMCD and neutron scattering) of magnetization across the DyFe2/YFe2 interfaces in low fields at 300 K. After cooling this simple structure to 12 K, the DyFe2 magnetization becomes pinned and the sample exhibits very large exchange bias (~2 T) and a large (35%) negative shift of the sample magnetization along the magnetization axis. However, when a large magnetic field is applied at room temperature, the magnetization adopts a spin-flop configuration across the DyFe2/YFe2 interfaces (confirmed with XMCD and neutron scattering). When cooled in a large field, the sample yields neither exchange bias nor a shift of the sample magnetization along the magnetization axis.

This work was supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS.

9:48AM X27.00010 In-plane anisotropy of NiCo multilayers, P. PANAYJIRAWUT, M.S. RZCHOWSKI, University of Wisconsin-Madison — We have grown NiCo magnetic multilayers on Si substrates by sputter deposition. The Ni$_{0.6}$Co$_{0.4}$ bilayer that repeats to form the multilayer ranges from 2 nm to 12 nm in thickness. The total multilayer thickness ranges from 50 nm to 75 nm. Room temperature vibrating sample magnetometer (VSM) measurements show that the multilayers have in-plane uniaxial magnetic anisotropy with K_u \sim 1.2x10^5 erg/cc. This is apparently induced during growth by the sputtering geometry, as we also see uniaxial in-plane anisotropy in individual 30 nm thick Ni (K_u \sim 0.3x10^5 erg/cc) and Co (K_u \sim 2.9x10^5 erg/cc) sputtered films. However the multilayer anisotropy is more complex as it arises from an interaction between the Ni and Co layers, with the Ni and Co layer magnetizations to first approximation rotating together.

10:00AM X27.00011 Determination of inhomogeneous magnetic profiles in an asymmetric Fe/Gd multilayer, EUGENY KRAVTSOV, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, SUZANNE G.E. TE VELTHUIS, YONGSEONG CHOI, J. SAMUEL JIANG, Materials Science Division, Argonne National Laboratory — We have studied the dependence of the detailed magnetization depth profile in a [Fe(35 A)/Gd(50 A)]$_n$ multilayer on the applied magnetic field and temperature. Utilizing the complementarity of x-ray resonant magnetic reflectivity (element-specificity and high spatial resolution) and polarized neutron reflectivity (large magnetic scattering cross sections), we applied a unified approach by simultaneous refinement and resolved the complex magnetization profiles. It was found that the small number of periods together with the asymmetric termination (Fe-top, Gd-bottom) lead to unique inhomogeneous magnetic phases, which are characterized by significant twisting of Fe and Gd magnetic moments and non-uniform distribution of magnetization density within the Gd layers.

1Work at Argonne is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

10:12AM X27.00012 Magnetic Compensation in Ferrimagnetic Bimetallic Oxalates1, PETER REIS, University of North Dakota and Oak Ridge National Laboratory, RANDY FISHMAN, FERNANDO REBOREDO, Oak Ridge National Laboratory, CUANNA MORENO, University of North Dakota — Bimetallic oxalates are layered organic magnets with the chemical formula A[M(II)M'(III)(ox)]$_n$, where M(II) and M'(III) are transition metal ions, A is an organic cation, and ox = C$_2$O$_4$. For some ferrimagnetic bimetallic oxalates, the magnetization changes sign at a compensation temperature below the ferrimagnetic transition temperature. We have initiated a systematic study of these compounds by examining the possibility of magnetic compensation for any possible combination of transition metal ions. Our model includes spin-orbit coupling for both M(II) and M(III) ions, the antiferromagnetic exchange between neighboring metal ions mediated by the oxalate bridges, and the effects of the ligand fields. Using mean-field theory, we predict candidates that may exhibit magnetic compensation for certain choices of the intercalated cation A.

1Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.

10:24AM X27.00013 Giant Negative Magnetization in a Class of Layered Molecular-Based Magnets1, RANDY FISHMAN, FERNANDO REBOREDO, Oak Ridge National Lab — Bimetallic oxalates are a class of layered molecular-based magnets with transition metals M(II) and M(III) coupled by oxalate molecules in an open honeycomb structure. Energy, structure, and symmetry considerations are used to construct a reduced Hamiltonian, including exchange and spin-orbit interactions, that explains the magnetic compensation and giant negative magnetization in some of the ferrimagnetic Fe(II)Fe(III) compounds. By shifting the Fe(II) ions with respect to the oxalate molecules, the organic cation between the magnetic layers alters the C$_2$-symmetric crystal field and the orbital angular momentum of the ground-state doublet at the Fe(II) sites. We provide new predictions for the spin-wave gap, the effects of uni-axial strain, and the optical flipping of the negative magnetization in Fe(II)Fe(III) bimetallic oxalates [1]. [1] R.S. Fishman and F.A. Reboredo, Physical Review Letters 99, 217203 (2007).

1Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.
10:36AM X27.00014 Effect of thermal fluctuation on the recoil loops of exchange-coupled nanocomposite magnets. CHUANBING RONG, YUZI LIU, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019 — Exchange-coupled hard/soft nanocomposite magnets have attracted great attention due to the very high potential energy product. One of the most effective ways to characterize the exchange-coupling strength in the nanocrystalline magnets is the measurement of recoil loops. It is often noted that the recoil curves are widely open for the hard/soft nanocomposite magnets but are narrow and even close for the single-phase magnets. In this work, we studied recoil loops of the FePt/Fe3Pt nanocomposite magnets. It was interesting to find that the parameter that describes the openness of the loops, $\Delta m_{rc}$, is significantly dependant on the sweep rate of applied field, especially for the nanocomposite magnets with high soft-phase content, where $\Delta m_{rc}$ is maximum difference between upper and lower magnetization curves of the recoil loops. The quantitative analysis shows a reciprocally linear relation between $\Delta m_{rc}$ and the activation volume, which means that the recoil loops are intimately related to the thermal fluctuation. The large open area of the nanocomposite magnets compared to that of single phase magnets is attributed to the more unstable magnetization process in the exchange-hardened soft phase.

10:48AM X27.00015 Effects of additives on hydrogen absorption and desorption characteristics of Nd(Fe,Mo)12 alloys. JINGZHI HAN, CHANGSHENG WANG, HONGLIN DU, HAIYING CHEN, YINGCHANG YANG, School of Physics, Peking University, 100871 — Effects of additives such as Co, Zr, Nb and Ga on hydrogen absorption and desorption characteristics of Nd(Fe,Mo)12 alloys are investigated. The results show that Zr or Nb addition increases the temperature of the disproportionation reaction and, Co or Ga addition reduces the temperature of the disproportionation. The corresponding D-H-HRD phenomena are discussed, and whether leading to anisotropic powders or not is suggested to be related to crystal growth direction of the Nd-Fe-B and Nd(Fe,Mo)12 system. However, according to the XRD measurement of the magnetic oriented samples, the anisotropic HDDR powders are not found. In order to analyze the reason leading to the anisotropic Nd(Fe,Mo)12 and anisotropic NdFe5B powders, the similarities and differences of the Nd(Fe,Mo)12 and NdFe5B systems and their corresponding HDDR phenomena are discussed, and whether leading to anisotropic powders or not is suggested to be related to crystal growth direction of the Nd-Fe-B and Nd(Fe,Mo)12 system. At the same time, it is also found that the Nb addition is helpful for improving the magnetic properties of the HDDR Nd(Fe,Mo)12 and NdFe5B magnetic materials, and the HDDR NdFe10.3Nb1.2Mo1.5X powders have a Br of 54 emu/g, a iHc of 3950 Oe. Moreover, the Mr/Ms ratio of the above powders reaches 0.60.

Friday, March 14, 2008 8:00AM - 10:48AM — Session X28 DMP: Focus Session: Optical Properties of Nanostructures VII: Surface Plasmons and Periodic Arrays — Morial Convention Center 220

8:00AM X28.00001 Plasmonic propagation along Metal/Semiconductor/Metal nanowires. LAETITIA BERNARD, MARLEEN H. VAN DER Veen, DANIEL TURNER-EvANS, ERIC R. DUFRESNE, MARK A. REED, Faculty of Engineering, Yale University, Kwan SKINNER, SEAN WASHBURN, Department of Physics and Astronomy, University of North Carolina — Recent advances demonstrated metallic nanowires as structures allowing selective coupling of photons to fluctuations in the surface density of electrons, and the propagation of these plasmon modes along the wire. We report here the observation of such propagating plasmons in heterogeneous metal/semiconductor/metal nanowires. Specifically, we excite one end of a Au/CdSe/Au nanowire with focused laser light and demonstrate the coupling of photons into the plasmon modes of the wire. These modes propagate along the wire, being emitted as elastically scattered photons, exclusively at the metal/semiconductor interfaces and the distal end. Through control of the excitation wavelength and wire composition, we gain insights about the nature of the plasmon propagation through CdSe, allowing direct comparison with standard metal studies. This contributes to the growing interest in plasmonics within nanoscale devices by extending it to semiconductor materials, and goes towards the integration of optics with nanotechnology.

8:12AM X28.00002 Plasmonic Interfaces for Electro-Optic Characterization of Molecular Junctions. MARLEEN H. VAN DER Veen, LAETITIA BERNARD, JASON MERRILL, ERIC R. DUFRESNE, MARK A. REED, Yale University — Metallic nanowires have interesting optical applications that make them promising platforms for sensing applications. The optical properties originate from the excitation of surface plasmon polaritons with light. We use this phenomenon to develop new spectroscopic tools to characterize the nature and details of the molecular structures with nanometer-scale devices. To achieve optical excitation at the nanometer-scale, we use a far field plasmon launching and emission technique based on nanowires coupled to molecular junctions. It is shown that plasmons can couple efficiently across small interfaces and can propagate along crossed nanowires. Furthermore, the light emitted as elastic scattered photons can be used to selectively couple light into the region of molecules for optical excitation. The possibility of doing local optical excitation of molecules simultaneously with their current-voltage measurements could lead to a new sensing platform for molecules based on plasmonic interfaces.

8:24AM X28.00003 Study of the absorption spectra of periodic hole arrays. DIMITRIOS KOUKIS, DANIEL ARENAS, SINAN SELCUK, A.F. HEBARD, D.B. TANNER, S.V. SHABANOV — The absorption of light by periodic hole arrays was studied for various open area fractions and wavelengths. We determined the absorption by measurements of the transmittance (T) and reflectance (R) at normal incidence and calculating the absorption as A = 1-R-T. The reflectance and transmittance were both measured, using a microphotometer in the near infrared region and Bruker IFS 113v in the mid-infrared region. Periodic hole arrays are characterized by "extraordinary" transmittance (larger than the predictions of geometrical optics) at frequencies just below the onset of first order diffraction by the periodic array. The absorption minimum occurs at frequencies slightly larger than the transmittance maximum. The absorption results for the various open area fractions were compared to theoretical predictions.
9:00AM X28.00006 Optical mapping of surface plasmon near-field spatial distribution in triangular silver nanostructures, ANDREW JONES, MATTHIAS RANG, University of Washington, BENJAMIN WILEY, Washington University, ZHI-YUAN LI, Institute of Physics, Chinese Academy of Science, YOUNAN XIA, Washington University, MARKUS RASCHKE, University of Washington — Plasmonic metal nanostructures have attracted interest in diverse fields including biomolecular sensing and nano-phononics. To understand the correlation of the optical response with the shape and size of the structure, we optically stimulate localized surface plasmons on chemically prepared Ag triangular nanostructures and utilize scattering-type Scanning Near-field Optical Microscopy (aSNOM) to map the optical near-field distribution with a spatial resolution down to 10nm. Using homodyne amplification allows for phase selective probing and identification of specific plasmon eigenmodes. For large triangles the superposition of several modes results in a complex distribution of the electric field whereas for smaller particles the distribution takes on a dipolar pattern.

9:12AM X28.00007 Photonic delocalization and optical propagation in one-dimensional random n-mer dielectric systems, RUWEN PENG, ZENG ZHAO, FENG GAO, LUSHUAI CAO, DE LI, ZHAN WANG, XIPING HAO, MU WANG, National Laboratory of Solid State Microstructures, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES TEAM — We have both theoretically and experimentally investigated the propagation of electromagnetic waves in a one-dimensional random n-mer (RN) dielectric system. Due to the positional correlation in the RN structure, the localization - delocalization transitions of photons happen at expected frequencies of photons. Multiple resonant transmissions are found in the photonic band gap. At each resonant mode, zero- Lyapunov exponent and undecayed field distribution of electromagnetic waves have been found through the whole system. Furthermore, the channel is opened for photonic transport at the resonant frequency, and the density of states of photons increases step by step as frequency increases. The theoretical results are experimentally demonstrated in RN dielectric multi-layer films of SiO2/TiO2 for visible and near infrared light.

9:24AM X28.00008 Quasiparticle dynamics and optical propagation in an optically-pumped microcavity far from equilibrium, PAUL EASTHAM, Imperial College London, RICHARD PHILLIPS, University of Cambridge — We propose and analyze a model for creating highly non-equilibrium quantum condensates from excitons and photons in a semiconductor microcavity on timescales shorter than any thermalization times. In a theoretical study of microcavity dynamics we show that a tailored optical pulse can directly create a supercooled exciton population by an analogue of adiabatic rapid passage. This state involves no macroscopic occupations and is thus not a condensate. At later times, however, it spontaneously develops into a quantum condensate far from equilibrium. This class of condensates encompasses phenomena similar to superradiance and lasing, but also includes states which give access to non-equilibrium Bose condensation in a solid-state system.

9:36AM X28.00009 Random Laser Emission from ZnO Nanocomposite Hybrids, A. STASSINOPoulos, S. H., ANASTASIADIS, D. G. PAPAZOGLOU, D. ANGLOS, Foundation for Research and Technology-Hellas, Greece, D. TSAGARAKIS, R. N. DAS, E. P. GIANNELIS, Cornell University — Highly scattering hybrid structures are produced either by incorporating ZnO nanoparticles in inert polymeric or inorganic sol-gel matrices or by depositing them on flexible substrates. All structures exhibit intense laser-like emission upon optical pumping. The ZnO particles provide both the gain and the strong scattering power, leading to photon localization due to multiple scattering. The polymer matrix offers ease of material fabrication and processability while the elastic substrate offers flexibility in view of potential applications. Excitation of the hybrids by laser pulses shows threshold behavior demonstrated by a dramatic increase in the emitted light intensity and significant spectral and temporal narrowing. We study the influence of pump pulse duration and sample temperature on the random laser efficiency whereas we measure the coherence length of the emission. Nanocomposite fabrication issues and pumping conditions are varied aiming at performance optimization and, thus, potential use of such materials in future light emission devices. Sponsored by the Greek GSRT, by NATO's Scientific Affairs Division and by the EU.

This work was supported by the EC Network of Excellence SANDIE, Contract No. NMP4-CT-2004-500101.
10:12AM X28.00012 Probing Bright and Dark Surface Plasmon Modes in Au Nanoparticles Using a Fast Electron Beam, MING-WEN CHU, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan, VIKTOR MYROSHNYCHENKO, F. JAVIER GARCÍA DE ABAJO, Instituto de Optica, CSIC Madrid, Spain, CHENG HSUAN CHEN, Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan, CENTER FOR CONDENSED MATTER SCIENCES, NATIONAL TAIWAN UNIVERSITY, TAIPEI, TAIWAN TEAM, INSTITUTO DE OPTICA, CSIC MADRID, SPAIN TEAM — We have studied the surface plasmons (SPs) of individual and coupled Au nanoparticles (NPs) with various sizes and shapes by electron energy-loss spectroscopy (EELS) using a 2-nm monochromatized fast electron beam in a scanning transmission electron microscope (STEM). EELS spectra were investigated with the beam in grazing incidence, the optical near-field setup, and bright SP modes (visible by light) were identified in both individual, coupled NPs ranging from near-IR to visible regimes. In an individual long rod with an aspect ratio of ~6, a dark SP mode invisible by light was surprisingly characterized, supported by calculations of the macroscopic dielectric responses. With the NPs coupling, rich bright, dark SP modes emerge and the suppression of one mode over the other is dictated by the beam position when approaching a geometrically centered site. The electron scattering geometry thus plays the role the SP-mode selection, never documented before.

10:24AM X28.00013 Quantum confined Stark effect in organic fluorophores, XIHONG PENG, Rensselaer Polytechnic Institute (RPI), JOHN ANDERSON, US Army Corps of Engineers, GARY TEPPER, SUPRIYO BANDOPADHYAY, Virginia Commonwealth Univ, SAROJ NAYAK, RPI — Fluorescent molecules have widely been used to detect and visualize structure and processes in biological samples due to its extraordinary sensitivity. However, the emission spectra of fluorophores are usually broad and the accurate identification is difficult. Recently, experiments show that energy shifts by Stark effect can be used to aid the identification of organic molecules [1]. Stark effect originates from the shifting/splitting of energy levels when a molecule is under an external electric field, which shows a shift/splitting of a peak in absorption/emission spectra. The size of the shift depends on the magnitude of the external field and the molecular structure. In this talk we will show our theoretical study of the peak shifts on emission spectra for a series of organic fluorophores such as tyrosine, tryptophan, rhodamine123 and coumarin314 using density functional theory. We find that a particular peak shift is determined by the local dipole moments of molecular orbitals rather than the global dipole moment of the molecule. These molecular-specific shifts in emission spectra may enable to improve molecular identification in biosensors. Our results will be compared with experimental data. [1]Unpublished, S. Sarkar, B. Kanchibotla, S. Bandopadhyay, G. Tepper, J. Edwards, Anderson, and R. Kessick.

10:36AM X28.00014 Effects of electron heating on femtosecond laser-induced coherent acoustic phonons, JINCHENG WANG, CHUNLEI GUO, University of Rochester — In this work, we employ a surface plasmon technique to resolve the dynamics of femtosecond laser-induced coherent acoustic phonons in noble metals. Clear acoustic oscillations are observed in our experiments. We further find that the initial phase decreases linearly with pump fluence. Our model calculations show that the hot electrons instantaneously excited by femtosecond pulses contributes to the generation of coherent acoustic phonons in metals.

Friday, March 14, 2008 8:00AM - 11:00AM – Session X29 DMP: Focus Session: Carbon Nanotubes and Related Materials XV: Electronic Structure and Optical Properties Morial Convention Center 221

8:00AM X29.00001 Saturation of Photoluminescence from Carbon Nanotubes at High Laser Intensities: Exciton-Exciton Annihilation near the Mott Density, YOICHI MURAKAMI, Rice University, The University of Tokyo, JUNICHIRO KONO, Rice University — We have carried out a nonlinear photoluminescence excitation (PLE) spectroscopy study of carbon nanotube ensembles using intense, femtosecond, and wavelength-tunable optical pulses. For all PL features we examined, their intensities were seen to saturate at high laser fluence, irrespective of whether the excitation was resonant or non-resonant with the E_22 transition. As the fluence was increased from the linear regime to the saturation regime, excitation resonances at E_22 energies gradually broadened and eventually became completely flat at the highest fluence, indicating that the PL intensity became independent of the excitation wavelength. However, the energies and lineshape of PL emission peaks did not show any changes throughout the entire range of fluence used. Through absorption spectroscopy at high laser intensities, we also demonstrated that E_22 absorption peaks do not show any shift or broadening even at high laser fluence, indicating that state-filling or scattering is not the cause of the observed “flattening” of the excitation spectra. We developed a model to explain these observations by carefully taking into account the spatial overlap of excitons when the average inter-exciton distance approaches the Bohr radius in the exciton-exciton annihilation process.

8:12AM X29.00002 Curvature Effects on the E_{23} and E_{44} Exciton Transitions in Semiconducting Single-Walled Carbon Nanotubes, STEPHEN DOORN, ERIK HARDOZ, Los Alamos National Laboratory, SERGEI BACHILO, BRUCE WEISMAN, Rice University — We discuss recent measurements of the E_{33} and E_{44} transitions of small diameter (0.7 to 1.2 nm) single-walled carbon nanotubes using deep blue (415 to 465 nm) resonance Raman spectroscopy and photoluminescence excitation spectroscopy in the UV and blue regions (280 to 480 nm). Individual radial breathing mode features, as well as Raman and photoluminescence excitation maxima, are assigned to specific nanotube chiralities. Transition-dependent trends in RBM intensities are discussed. We present a scaling law analysis of transition energies and show that energies for nanotubes with diameter less than 0.9 nm are not explained by previous scaling law descriptions for larger diameter nanotubes. This new behavior at small diameters is interpreted in terms of both a crossing-over of the E_{33} and E_{44} trend lines for a given 2n-m branch, and a chirality dependence in the many-body exciton effects that becomes significant at high curvatures.

8:24AM X29.00003 Exciton binding energies in metallic single-walled carbon nanotubes are comparable to those in semiconducting ones, ZHENDONG WANG, SUMIT MAZUMDAR, University of Arizona — Excitons in metallic single-walled carbon nanotubes (M-SWCNTs) have attracted both theoretical and experimental attention recently. It has been claimed that exciton binding energies in M-SWCNTs are of an order of magnitude smaller than those in semiconducting single-walled carbon nanotubes (S-SWCNTs). We have investigated M-SWCNTs within a two-electron Hamiltonian that has previously reproduced quantitatively the absolute energies as well as the binding energies of both longitudinal and transverse excitons in S-SWCNTs. We are able once again to reproduce quantitatively the available absolute exciton energies and the optical absorption spectra of M-SWCNTs with diameters 0.9 - 1.4 nm. While we need a dielectric constant larger than in the S-SWCNTs, our calculated exciton binding energies in this diameter range are 0.2 - 0.3 eV, only slightly smaller than those in S-SWCNTs with similar diameters.

2F. Wang et al., unpublished
5Supported by NSF-DMR-0705163.
1. Fagan et al. 2. Shaver et al. Our observations exchange-split bright and dark exciton bands with Aharonov-Bohm-phase-dependent energies, masses, and oscillator strengths, which successfully reproduces states, making the triplet state optically active. Supported by ONR (No. N00014-06-1-0228) and NSF.

 observable Zeeman splitting, or for the dark exciton to be observed. We instead suggest that the EuS provides spin orbit coupling to mix the singlet and triplet its position shifts by approximately 7 meV. From this we estimate that the EuS layer produces an effective magnetic field of 7 T. This is too small to produce so that the spin-up level lies 0.36 eV below the spin-down level. We monitor the nanotube photocurrent at 4.2K for magnetic fields between 0 and 50 mT.

 for carbon nanotubes are not observable under normal conditions, including the so-called dark excitonic states and the spin triplet states. Here, we develop a theoretical model of one-dimensional magneto-excitons, based on recently-proposed of the form of the diffusion coefficient assuming exciton-phonon coupling as the underlying mechanism will be discussed.

 This work was supported by grants from the National Institutes of Health P41-RR05969, and NSF CCR 02-10843.

 1. O. N. TORRENS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, M. ZHENG, DuPont CR&D — Phonon sideband optical spectroscopy determines the energy of the dark \( K \)-momentum exciton for (6,5) carbon nanotubes (CNTs). One-phonon sidebands appear in absorption and emission, split by two zone-boundary (\( K \)-point) phonons. Their average energy locates the \( E_{11} \) \( K \)-momentum exciton 36 meV above the \( E_{11} \) bright level, higher than available theoretical estimates. A model for exciton-phonon coupling shows the absorption sideband depends sensitively on the \( K \)-momentum exciton effective mass and has minimal contributions from zone-center phonons, which dominate the Raman spectra of CNTs.

Supported by NSF MRSEC DMR-0520020.


 10:00AM X29.00009 Dark excitons in single-walled carbon nanotubes investigated by electroabsorption spectroscopy, HIDEO KISHIDA, Y. NAGASAWA, S. IMAMURA, A. NAKAMURA, Department of Applied Physics, Nagoya University, Japan — We report electroabsorption (EA) spectra in micelle-wrapped single walled carbon nanotubes (SWNT). By applying the high electric field (up to 85kV/cm), the absorption spectra of semiconducting SWNTs show field-induced change in the region of \( E_{11} \) and \( E_{22} \) transitions. The EA spectra are essentially reproduced by the second derivative curves of the absorption spectra. Such spectral features indicate that the bright (one-phonon allowed) exciton and dark (two-phonon allowed) exciton for each chiral index are nearly degenerate. The closer scrutiny of the EA spectra reveals that the dark excitons for several chiral indices are located on the higher energy side of the bright states.

 10:12AM X29.00007 \( K \)-momentum dark exciton energy in carbon nanotubes, O. N. TORRENS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, 19104 — We observe room temperature, sub-Tesla magnetic field effects on the photoluminescence of aqueous suspensions of single-walled carbon nanotubes and on the electrical transport of carbon nanotube composites. The nearly identical field scale found in both cases suggests a common origin for the phenomena. In aqueous suspensions, weak magnetic fields decrease the nanotube photoluminescence intensity by \( \sim 0.1\% - 1\% \), an effect which saturates by \( \sim 1 \) Tesla. We explore this magnetic darkening as a function of surfactant, magnetic field and direction, temperature, and nanotube chirality. For carbon nanotube epoxy composites and aerogels, low magnetic fields produce a similar decrease in the device resistivity, which is found to be temperature dependent. We discuss these new magnetic field effects in the context of excitonic magneto physics and magnetic field effects observed in other organic semiconductor systems.

Supported by NSF MRSEC DMR-0520020.

 1. O. N. TORRENS, J. M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA — We have investigated excitons in semiconducting single-walled carbon nanotubes (SWNTs) through low-temperature magneto-photoluminescence (PL) of highly-aligned SWNT films in magnetic fields (B) up to 55 T. The magnetic field was generated using the 60 T long pulse magnet powered by a 1.4 GVA motor-generator at the National High Magnetic Field Lab in Los Alamos, NM. Polyacrylic acid films containing DNA suspended CoMoCAT SWNTs were stretch-aligned, and the alignment factor was analyzed by polarized Raman spectroscopy. Utilizing two well-defined measurement geometries, SWNT || B and SWNTs \( \perp \) B, we provide unambiguous evidence that the PL from excitons in SWNTs is sensitive only to the B-component parallel to the tube axis. We developed a theoretical model of one-dimensional magneto-excitions, based on recently-proposed exchange-split bright and dark exciton bands with Aharonov-Bohm-phase-dependent energies, masses, and oscillator strengths, which successfully reproduces our observations.

10:36AM X29.00012 Free Carrier Auger Relaxation of Excitons in Carbon Nanotubes, JESSE KINDER, EUGENE MELE, University of Pennsylvania — We study a relaxation pathway in doped carbon nanotubes in which optically pumped excitonic states interact with free electrons or holes through an Auger process. The exciton recombines nonradiatively, transferring its energy and momentum to a free carrier. The calculated decay rate depends on temperature, exciton density, and the amount of doping. For optically excited bright excitons, conservation of energy and momentum forbid this decay below a critical doping density. For the heavier dark excitons, recombination is allowed for any nonzero doping density. By studying the phase space for this Auger process and exciton-exciton annihilation, we find that the free carrier interaction can dominate the relaxation rate at low exciton densities.

10:48AM X29.00013 Magnetic Brightening of Dark Excitons in Individual Single-Walled Carbon Nanotubes1, A JIIT SRIVASTAVA, JUNICHIRO KONO, Rice University, HAN HTOON, VICTOR I. KLIMOV, Los Alamos National Laboratory — We have performed micro-photoluminescence (PL) studies on individual single-walled carbon nanotubes (SWNTs) at varying temperatures (T = 4 K – 100 K) in magnetic fields (B) up to 5 T, which provide direct evidence for the existence of dark excitons in SWNTs. Only when the B was parallel to the tube axis, we observed the appearance of a secondary peak at a lower energy with respect to the main emission peak. The secondary peak increased in intensity with increasing B at the expense of the main peak. At the lowest T, a complete reversal of emission intensity from the main peak to the side peak was seen as the B was increased. However, the main peak was recovered as the T was increased at a fixed B. These behaviors can be explained by assigning the main and secondary peaks to the lowest-energy bright and dark singlet exciton states, respectively. The absence of these behaviors in B perpendicular to the tube axis convincingly suggests that brightening is induced by the Aharonov-Bohm phase. The zero-field dark-bright splitting is found to be ~1.2 meV, which is lower than most theoretical predictions.

1This work was supported by ARO through Grant No. 49735-PH.

Friday, March 14, 2008 8:00AM - 10:48AM — Session X30 DCMP: Composite and Porous Media Morial Convention Center 222

8:00AM X30.00001 Modeling of multiscale porous media, B. BISWAL, ICP, University of Stuttgart, Germany, P.-E. OREN, Numerical Rocks AS, Norway, R.J. HELD, StatoilHydro ASA, Norway, S. BAKKE, Numerical Rocks AS, Norway, R. HILFER, ICP, University of Stuttgart, Germany — A continuum geometrical model for reconstructing three dimensional pore scale microstructure of multiscale porous media is presented. Pore scale geometries of different carbonate textures are successfully reconstructed with informations from thin sections. The reconstructed models incorporate correlations with the primordial depositional textures, scale dependent intergranular porosity over many decades, vuggy porosity, a percolating pore space, a fully connected matrix space, strong resolution dependence and wide variability in the permeabilities and other properties. A method to generate synthetic micro-CT images at arbitrary resolution is also developed. The model can be extended to a wide class of multiscale porous media.

1This research was funded by StatoilHydro ASA.

8:12AM X30.00002 Direct observation of pore blocking and advanced adsorption in nanoporous alumina: cooperative effects at the origin of hysteresis1, FELIX CASANOVA, CASEY E. CHIANG, University of California San Diego, CHANG-PENG LI, University of Michigan, IVAN K. SCHULLER, University of California San Diego — We tailor anodized alumina with independent pores with well-defined, simple geometries (inkbottle, funnel), in order to study the effects of pore morphology in hysteretical capillary condensation, independently from other cooperative processes such as network effects. We confirm, by direct observation using optical interferometry, the occurrence of two cooperative phenomena: the classical pore blocking effect in nearly ideal 'inkbottle' pores (which has usually been employed to describe hysteresis loops in disordered interconnected porous materials) and the advanced adsorption in pores with a change in the cross section. Both effects have been predicted in theoretical and simulation works, but not directly observed experimentally before. They are relevant for the development of a theory of the poorly understood hysteresis in complex porous materials.

1Supported by AFOSR and Spanish MEC-Fullbright.

8:24AM X30.00003 Acoustic Band Pass, Band Gap and Dispersion in Discrete Media at Micro and Nano Scales, HASSON TAVOSSI, Valdosta State University — Acoustic properties of models of crystals, when measured at macroscopic scale, are found experimentally to have remarkable similarities with the same wave properties observed at atomic and nano-scales. It can be shown that, elastic moduli and other wave properties such as; band-pass, forbidden band, wave tunneling, attenuation, cutoff-frequency, and dispersion, depend on the similar structural factors as for phonons in crystals. Acoustic properties of the macroscopic models of discrete media, in the length scale range; 1.5 mm to 30 micrometers, and the frequency range; audible to ultrasonic are studied. The Band-pass, band-gap, attenuation, and dispersion expressed in wave-number (ka), show similar characteristics as the phonons in solids. These findings can lead to a better understanding of the wave properties of solids at nanoscales. The readily analyzable wave models at large scale are convenient tools to verify experimentally the models for complex binary composites. Experimental findings and numerical results for wave properties of discrete structures at large scale are compared with atomic scale wave behavior of solids, for a wide range of frequencies, from audible to ultrasound, to show the common characteristics with the phonons behavior in solids.
8:36AM X30.00004 Conducting-tip AFM Studies of Multi-Walled Carbon Nanotube/Polymide Nanocomposites, A. TRIONFI, D. SCRYMGEOUR, J.W.P. HSU, Sandia National Laboratories, M.J. ARLEN, D. WANG, L.-S. TAN, R.A. VAIA, Air Force Research Laboratory — Electrical transport studies of multi-walled carbon nanotube (c-MWNT)/polymer nanocomposites have shown metallic behavior with conductivity $\sigma = \sigma_0 (\phi^2 - \phi)^3$ above the percolation threshold. The conductivity depends on three aspects of the conducting network (CN): the conductivity of the constituent c-MWNT, the number of c-MWNT making up the CN, and the detailed interconnectivity of the CN. Conducting-tip atomic force microscopy (C-AFM), we have studied the density and conductivity of the c-MWNT CN as a function of c-MWNT loading between 0.5 - 5.0 wt % in a polymide matrix. Using the Principle of Delese, the volume fraction of the c-MWNT CN can be calculated from the conducting areal density measured in the C-AFM scans. The results of the C-AFM tests have shown localized areas of electrical transport associated with c-MWNT as well a clear dependence of conducting areal density and conductivity on the c-MWNT loading. This work was performed in part at the US Department of Energy, Center for Integrated Nanotechnologies, at Los Alamos and Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

8:48AM X30.00005 Systematic Study of Microwave Absorption, Heating, and Microstructure Evolution of Porous Carbon Powder Metal Compacts, DARIN ZIMMERMAN, JOHN DIEHL, EARNIE JOHNSON, KELLY MARTIN, NICHOLAS MISKOVSKY, CHARLES SMITH, GARY WEISEL, BROCK WEISS, The Pennsylvania State University, Altoona College, JUNKUN MA, Southeastern Louisiana University — We present a systematic study of the absorption, heating behavior, and microstructure evolution of porous copper powder metal compacts subjected to 2.45 GHz microwave radiation and explain our observations using known physical mechanisms. Using a single mode microwave system, we place the compacts in pure electric (E) or magnetic (H) fields and compare the heating trends. The observed trends in the E- and H-field heating reflect the dramatic changes in the conductivity, permittivity, and permeability of the samples caused by the microstructure evolution during heating in the two types of fields. The observed dependence of the initial microwave heating of the samples suggests that the microwave absorption in the sample is dominated by the properties of the individual metal particles composing the sample.


9:00AM X30.00006 Do pores strengthen materials? – A pore size effect analysis, CATALIN PICU, MOHAN NUGGehally, MARK SHEPHERD, Rensselaer Polytechnic Institute — Pores with radius larger than several microns are known to reduce the yield and flow stress of ductile materials and to increase their toughness. In this work we discuss a new mechanism leading to an increase in the strength of a material by nanosized pores. We show that voids grow by the emission of dislocations. As the void radius is reduced, while their volume fraction is kept constant, the mean spacing between voids decreases and their number increases. This makes the concurrent dislocation nucleation from neighboring voids more difficult. The situation is equivalent to increasing the density of dislocation sources in the material. Furthermore, we show that the critical stress for dislocation nucleation form an isolated void also increases as the pore size is reduced. The analysis is performed using a computationally efficient adaptive atomistic-continuum method.

9:12AM X30.00007 First-Principles Calculations for the Dislocations in Titanium Nitride, RAMKUMAR GUDIPATI, University of Tulsa, Y.G. SHEN, City University of Hong Kong, WENTAO XU, University of Kentucky, A.S. RAO, H.L. DANG, SANWU WANG, University of Tulsa — Nanostructured superhard materials have been successfully synthesized in recent years. The hardness of nanosuperlatticess and nanocomposites significantly exceeds that of the component materials. While it is believed that the nanodimensions are needed to impede dislocation activity and grain-boundary sliding, relevant calculations are rare. We report first-principles density-functional calculations for the core structures and energetics of various dislocations including the [110], [110], [111], [110][100], [100][100] and [100][110] edge dislocations in bulk TiN. We found that the formation energies of the core dislocations were continuously increased when their sizes decreased. We also found that the most common types of dislocations in TiN are the [110][110] and [110][111] edge dislocations. The obtained results are helpful for elucidating the atomic-scale mechanism for the superhardness of nanocomposites.

1Supported by the National Science Foundation (CMS-0510057 and CMMI-0645953).

9:24AM X30.00008 Interaction of RDX Explosive Molecules with Metal-Organic, KHORGOLKHUU ODBADRakh, JAMES LEWIS, West Virginia University — We have studied interactions of cyclotrimethylene trinitramine (RDX), a highly energetic explosive molecule, with metal-organic framework of composition Zn$_2$ O$_2$ (1,4-benzene dicarboxylate)$_3$ (MOF-5), within ab initio density functional theory method. The structures were optimized with the Fireball atomic orbital basis sets to a good agreement with experimental values. Optimal surface geometries have been obtained for MOF-5-RDX system and first principles estimates of the binding energies, charge transfer, and activation barriers are given.

1NSF 07-528
2corresponding author

9:36AM X30.00009 Control of Microcellular Structure in Polymeric Foams via Nanofiller Size and Surface Chemistry, KEREM GOREN, LINDA SCHADLER, RAHMI OZISIK, Rensselaer Polytechnic Institute — Polymeric foams are used in many applications, where thermal insulation, selective sound inhibition or low density materials are needed. They are generally produced by blending polymer with a chemical blowing agent, which releases inert gas at processing temperatures. There are two major drawbacks to this process: chemical residues that form during the decomposition of blowing agent and formation of large (macroporous) pores that weaken the material. To overcome these drawbacks, supercritical carbon dioxide (scCO2) is used. Use of scCO2 along with nanofillers provide heterogeneous nucleation, and present the opportunity to control pore size and pore distribution. In the current study, the effect of silica size and silica-scCO2 interaction on microcellular structure was investigated. Two different silica fillers were synthesized: 15 and 150 nm. These silica nanofillers were surface modified with tridecafluoro-1,1,2,2-tetrahydrooctyl triethoxysilanes. Dynamic Light Scattering, FT-IR, TGA, and SEM were used to characterize the samples. Results indicate that there is a strong correlation between surface chemistry, and hence scCO2 and filler interaction on pore size and size distribution.

1This material is based upon work supported by the National Science Foundation under Grant CMMI-0500324.
9:48AM X30.00010 Diffusion in an array of cavities in two and three dimensions . MYKYTA V. CHUBYNSKY, FRANCIS TORRES, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — We consider diffusion of point-like particles in arrays of cavities separated by infinitely thin walls with holes. We show that in the small-hole limit, the effective diffusion coefficient $D$ is related to the electrical capacitance of a plate of the same shape as the hole. Applying this result to elongated holes in 3D, we find an interesting logarithmic dependence of $D$ on the hole width. A logarithmic dependence is also obtained in 2D. As a consequence, the diffusion rate reaches 10% of the free diffusion rate when the hole widths are only about $10^{-6}$ of the cavity size. The theoretical predictions are validated using a numerically exact computational method. In the opposite limit, where holes span the cavity boundaries nearly completely and only small pieces of walls remain, analytical calculations are also possible. The result in this case is interesting, since a finite reduction in the diffusion coefficient is obtained even for infinitely thin walls, contrary to predictions of various effective-medium theories that this reduction should be proportional to the excluded volume fraction.

10:00AM X30.00011 First principles modeling of structure and properties of multi-component amorphous steels , VIATCHESLAV KAZIMIROV, DESPINA LOUCA, University of Virginia, MICHAEL WIDOM, Carnegie Mellon University, MICHAEL WIDOM COLLABORATION — Amorphous steels (iron based metallic glasses) exhibit unique physical properties that have opened the venue to new commercial applications as well as renewed the interest in this field. To provide a realistic description of the three dimensional structures and associate the coordinated environment of atoms to physical properties, first principles quantum mechanical molecular dynamics (MD) simulations along with the pair density function (PDF) analysis of neutron and X-ray diffraction data were used by way of considering chemical effects, ionic size ratio and concentration. Direct comparison of the simulated atomic structures obtained from MD with the local atomic structures determined experimentally show a very good agreement between the two, indicating that this theoretical approach can be applied towards simulating multi-component alloys. The atomic coordinates were used to develop the building blocks of cluster-like structures that give rise to the short-range order. The diffusion rates of different atom species were modeled at several temperatures that allowed us to describe the quenching process. In addition, the bulk moduli as a function of chemical composition were simulated and showed a very good agreement with the ones obtained experimentally.

10:12AM X30.00012 Structural, dynamic and electronic properties of amorphous Al$_2$O$_3$: ab-initio molecular dynamics calculations$^1$. GONZALO GUTIERREZ, University of Chile, Chile, SERGIO DAVIS, Royal Institute of Technology, Sweden — First principles molecular dynamics (MD) calculations of amorphous Al$_2$O$_3$ in a system consisting of a supercell of 80 atoms is reported. A detailed analysis of the interatomic correlations allows us to conclude that the short range order is mainly composed by AlO$_4$ tetrahedra, but in contrast to classical MD results, also an important number of AlO$_2$ units are present. The vibrational density of state, calculated by means of the velocity autocorrelation function, present two main bands, a low frequency one related to the inter-tetrahedron vibration and a high frequency band related to the intra-tetrahedron vibration. By means of a geometry relaxation we obtain a fully relaxed system, and calculated its elastic properties. The reported bulk modulus is 193.4 GPa, the smallest among the several phases of alumina. The electronic properties were characterized by means of both the total and partial electronic density of states as well as by means of the electron localization function. The system present a rather small gap of 2.4 eV. The consequences of these results will be discussed.

$^1$Grant Anillo ACT/24-Chile.

10:24AM X30.00013 Disorder Induced Transition into a One-Dimensional Wigner Glass. SHIMUL AKHANJEE, JOSEPH RUDNICK, UCLA — The destruction of quasi-long range crystalline order as a consequence of strong disorder effects is shown to accompany the strict localization of all classical plasma modes of one-dimensional Wigner crystals at $T = 0$. We construct a phase diagram that relates the structural phase properties of Wigner crystals to a plasmon delocalization transition recently reported. Deep inside the strictly localized phase of the strong disorder regime, we observe “glass-like” behavior. However, well into the critical phase with a plasmon mobility edge, the system retains its crystalline composition. We predict that a transition between the two phases occurs at a critical value of the relative disorder strength. This transition has an experimental signature in the AC conductivity as a local maximum of the largest spectral amplitude as function of the relative disorder strength.

10:36AM X30.00014 Structural and electronic properties of amorphous silicon carbide: A first principles and experimentally constrained molecular relaxation approach$^1$. PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAYMOND ATTA-FYNN, University of Texas at Arlington — We present first-principles modeling of amorphous silicon carbide within a localized basis density functional formalism to study the electronic, vibrational and structural properties for system containing 10000 atoms. Our work for Si$_{50}$-C$_{50}$ system shows that the short range chemical order is dominated by heteronuclear Si-C bonds with coordination defect with a degree of chemical disorder. We calculate the electronic density of states that shows a presence of clean optical gap in the spectrum and study the localization nature of the electronic band tail states and vibrational eigenstates. We compare our results with existing models and experimental data available in the literature. Finally, we presents some preliminary results for models obtained by experimentally constrained molecular relaxation technique [1,2] that directly uses experimental data in conjunction with a classical force-field.

$^1$University of Southern Mississippi, Grant No. DE00945.
8:00AM X31.00001 Metallic Spin Liquid Behavior and Unconventional Anomalous Hall Transport of the Geometrically Frustrated Kondo Lattice Pr$_2$Ir$_2$O$_7$ — SATORU NAKATSUI, Institute for Solid State Physics, University of Tokyo — Among metallic magnets on geometrical frustrated lattices, the pyrochlore oxide Pr$_2$Ir$_2$O$_7$ is unique for its metallic spin liquid behavior and unconventional Hall transport phenomena. Despite the Weiss temperature $T^\ast = 20$ K due to the RKKY interaction, Pr$_2$Ir$_2$O$_7$ exhibits no magnetic long range order, but spin freezing at a very low temperature $\sim 120$ mK. Instead, the Kondo effect, including In$^T$ dependence in the resistivity, emerges and leads to partial screening of the $J_1$-moments below $T^\ast$. Moreover, the underscreened 4f-moments show spin-polarization behavior below a renormalized energy scale of $\theta_{\text{K}} \sim 1.7$ K. Interestingly, in this spin-fluid-like paramagnetic regime, the Hall resistivity $\rho_{xy}$ becomes largely enhanced, and shows behavior far different from anomalous Hall effects (AHE) due to the spin-orbit coupling observed in ordinary magnetic conductors. We discuss the origin of the metallic spin liquid behavior and unconventional AHE in terms of the spin chirality due to the non-coplanar texture of the $<111>$ Ising-like Pr moments. This work is based on the collaboration with Y. Machida, T. Tayama, T. Sakakibara (ISSP, Univ.of Tokyo), Y. Maeno (Kyoto Univ.), S. Onoda (RIKEN, Tokyo), C. Broholm (Johns Hopkins Univ.), C. Stock and J. van Duijn (ISIS), L. Balicas (NHMFL), Jung Young Cho, and Julia Y. Chan (Louisiana State Univ.).

This work is partly supported by Grant-in-Aid for Scientific Research on Priority Areas (190520019052003).


8:36AM X31.00002 Magnetic phase diagram of (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ (0 $\leq$ x $\leq$ 1.0) — Z.Q. MAO, Tulane University (TU), Z. QU, TU, L. SPINU, University of New Orleans, J. PENG, T.J. LIU, D. FOBES, TU, V. DOBROSAVLJEVIC, NHMFL and Florida State University, H.Q. YUAN, W. BAO, Los Alamos National Laboratory, J.W. LYNN, National Institute of Standards and Technology — The layered ruthenates (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ have received widespread attention in recent years since they display a remarkable range of unique superconducting and magnetic properties, such as spin triplet superconductivity and metamagnetic quantum criticality. We have recently studied properties of the double layered (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ solid solution series and established the magnetic phase diagram of this system using the high-quality single crystals grown by floating-zone method. We have observed rich magnetic ground states in this system: (I) itinerant metamagnetic state (0.08 $\leq$ x $\leq$ 0.4); (II) enhanced PM state accompanied by non-Fermi liquid behaviors near x $\sim$ 0.08; (III) ferromagnetic cluster glass (CG) phase featuring an extremely large Wilson ratio (~120) and enhanced electron correlation (0.40 $\geq$ x $\geq$ 0.08); (IV) long-range AFM state (1 $\geq$ x $\geq$ 0.40). Furthermore, we found a new phase which shows an unconventional anomalous Hall effect in a low temperature range immediately above the CG phase. The magnetization of this phase is found to follow a new scaling expression derived by phenomenologically extending the quantum Griffiths phase model.

8:48AM X31.00003 ARPES Investigations of the Electronic Structure Evolution of the Doped Ruthenate (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ — WILLIAM DUNKEL, Stanford University, FELIX BAUMBERGER, MILAN ALLAN, University of St. Andrews, WORAWAT MEEVASANA, Stanford University, ZHIQIANG MAO, Tulane University, ZHI-XUN SHEN, Stanford University — The bilayer ruthenate system (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ can be grown in the full range of dopings with the end members being an antiferromagnetic “bad metal” (x=1) and a paramagnetic Fermi liquid displaying a metamagnetic transition under applied field (x=0). Recent transport and magnetization measurements have shown that the system displays disorder-induced unconventional quantum critical behavior near the doping level x~0.3. We present ARPES data for a range of dopings to investigate the associated electronic structure evolution.

9:00AM X31.00004 Study of the Layered Perovskite Sr$_3$Ru$_2$O$_7$ by STS and ARPES — MILAN ALLAN, J. LEE, University of St. Andrews, UK, Cornell University, M. WANG, A. SCHMIDT, Cornell University, F. BAUMBERGER, A. TAMAI, J. FARRELL, University of St. Andrews, UK, C. Stock and J. van Duijn (ISIS), L. Balicas (NHMFL), Jung Young Cho, and Julia Y. Chan (Louisiana State Univ.) — The Ruddlesden-Popper series, Sr$_{n+1}$Ru$_n$O$_{3n+1}$ exhibits a variety of electronic phases, including triplet superconductivity (n=1) or metamagnetism (n=2). Here we report studies of the electronic structure of the bilayered perovskite Sr$_3$Ru$_2$O$_7$ (n=2) by means of scanning tunneling spectroscopy. Special attention is given to the influence of titanium impurity atoms on the local electronic structure. A comparison with angle resolved photoemission experiments on the same set of samples is drawn.

9:12AM X31.00005 Quasi-3D ordered lattice modulations in a bilayer ruthenate with no long-range order — ZAHRIRUL ISLAM, Argonne National Laboratory (ANL), ZHE QU, Tulane University (TU), YEJUN FENG, JONATHAN LANG, ANL, JIN PENG, ZHIQIANG MAO, TU — Bulk measurements reveal disorder-induced unconventional quantum critical behaviors in (Sr$_{1-x}$Ca$_x$)$_3$Ru$_2$O$_7$ (SCRO) compounds, in particular, near x $\sim$ 0.3. Here we report X-ray scattering studies on SCRO with x = 0.3, as well as those for the end members. We find that at x = 0.3 robust 2-unit-cell periodic lattice modulations exist that are characterized by ($\frac{1}{2}$, 0, 0) and ($\frac{1}{2}$, $\frac{1}{2}$, 0), respectively, even at room temperature. These modulations are transversely polarized and quasi-3D ordered in that they are fully coherent in the basal plane with c axis correlations at least one unit cell in extent. These modulations are due to correlated displacements of the O atoms. The displacement pattern is consistent with 2q modes of distortion of RuO$_6$ octahedra, signifying the presence of lattice and orbital correlations, although no long-range magnetic or orbital order is present. These modulations are absent in the end members.

1. Use of the Advanced Photon Source is supported by the DOE, Office of Science, Contract No. DE-AC02-06CH11357. Work at TU is supported by NSF under DMR-0645305, by DOE under DE-FG02-07ER46358, and the Research Corporation.

9:24AM X31.00006 Doping-Induced Structural and Physical Properties Changes in Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$ Single Crystals — BIAO HU, Univ. of Tennessee, Knoxville, TN 37996, MANUEL ANGST, Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, OVIDIU GARLEA, Neutron Scattering Science Division, ORNL, Oak Ridge, TN 37831, V.B. NASCIMENTO, Univ. of Tennessee, Knoxville, TN 37996, DAVID MANDRUS, Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, E.W. PLUMMER, Univ. of Tennessee, Knoxville, TN 37996 and Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, R. JIN, Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831 and Univ. of Tennessee, Knoxville, TN 37996 — In the homologous strontium ruthenate systems Sr$_{n+1}$Ru$_n$O$_{3n+1}$, double-layered Sr$_3$Ru$_2$O$_7$ exhibits unique physical properties. However, the partial substitution of Ru by the smaller Mn was found to change its ground state from a paramagnetic metal to an antiferromagnetic insulator with less distorted crystal structure. Interestingly, our Hall effect measurements show no change in the carrier concentration (x $\leq$ 0.2), suggesting that Mn is isovalent with Ru in Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$. This is further supported by the magnetization data, which yield effective spin S = 3/2 for Mn corresponding to Mn$^{+\frac{3}{2}}$. In addition to bulk physical properties, the doping dependence of the surface structure and lattice dynamics of Sr$_3$(Ru$_{1-x}$Mn$_x$)$_2$O$_7$ single crystals will be discussed.
9:36AM X31.00007 Relation between structure and magnetic properties in (Sr$_{1-x}$Ca$_{x}$)$_3$Ru$_2$O$_7$\textsuperscript{1} , J. PENG, Tulane University (TU). Z. QU, TU, L. SPINU, University of New Orleans, T.J. LIU, D. FOBES, Z.Q. MAO, TU — The (Sr$_{1-x}$Ca$_{x}$)$_3$Ru$_2$O$_7$ solid solution series exhibits rich magnetic ground states, ranging from itinerant metamagnetism, ferromagnetic instability, ferromagnetic cluster glass, to antiferromagnet.\textsuperscript{[1]} In this talk, we report a study on the relation between structure and magnetic properties in (Sr$_{1-x}$Ca$_{x}$)$_3$Ru$_2$O$_7$. Our Rietveld refinement of x-ray scattering data shows that the rotation angle of RuO$_6$ octahedra increases with increasing $x$, and approaches saturation for $x > 0.2$. The orthorhombicity, which is caused by the tilting of RuO$_6$ octahedra, occurs for $x > 0.4$ and enhances significantly for $x > 0.7$. By comparing these structural characteristics with the magnetic properties, we conclude that the ferromagnetic instability originates from the RuO$_6$ octahedra rotation, and the tilting of RuO$_6$ octahedra causes a significant magnetic anisotropy.\textsuperscript{[1]} Z. Qu et al. arXiv:0708.1291 (2007).

\textsuperscript{1}Work at Tulane is supported by NSF, DOE and the Research Corporation. Work at UNO is supported by DARPA.

9:48AM X31.00008 QPI in Sr$_3$Ru$_2$O$_7$ , JINHO LEE, University of St. Andrews, Cornell University, M. WANG, Cornell University, M. ALLAN, University of St. Andrews, A. SCHMITZ, Cornell University, F. BAUMBERGER, A. TAMAI, J. FARRELL, University of St. Andrews, J. C. DAVIS, Cornell University, Brookhaven National Laboratory, A. MACKENZIE, University of St. Andrews — Sr$_{n+1}$Ru$_n$O$_{3n+1}$ family drew substantial attention recently due to its plethora of electronic phases like triplet superconductivity or metamagnetism. Sr$_3$Ru$_2$O$_7$ (n = 2) is very similar to the triplet superconductor Sr$_3$Ru$_2$O$_4$ in 2D conductivity as well as in structure, but shows no superconductivity. Understanding of the underlying band structure is the first step to fathom this strongly correlated oxide. STM has proven to be a high precision tool to measure band dispersions in momentum space along with the atomically resolved real space spectroscopic properties. Here we report the first atomically resolved 2D spectroscopic maps in Sr$_3$Ru$_2$O$_7$ where QPI patterns are observed and discuss the band landscape responsible for the QPI in this energy range.

10:00AM X31.00009 Orbital Hierarchy Inversion and Magnetic Transition in Mn Doped Sr$_4$Ru$_3$O$_7$\textsuperscript{1} , MUHAMMED HOSSAIN, University of British Columbia, M.W. HAVERKORT, Z.H. HU, T. BURNUS, C.F. CHANG, S. KLEIN, J.D. DENLINGER, H.-J. LIN, C.T. CHEN, R. MATHIEU, Y. KANEKO, Y. TOKURA, S. SATOW, Y. YOSHIDA, H. TAKAGI, A. TANAKA, I.S. ELFIMOV, G.A. SAWATZKY, L.H. TJENG, A. DAMASCHELLI — Oxidine ruthenates are very important class of compounds that are extremely sensitive to impurities. Here we present a study of the Mn doped Sr$_4$Ru$_3$O$_7$ by X-ray Absorption Spectroscopy (XAS) and a combination of density functional theory (LSDA) and cluster calculations. We find that delocalized RuO matrix forces the Mn impurities to behave as a negative charge transfer system and donate a hole. As a result Mn impurities behave as Mn$^{3+}$ acceptors. Our XAS data clearly shows that the occupied $e_g$ orbitals have an in-plane alignment: a very surprising result in a tetragonally distorted system elongated along the c-axis. LSDA calculations reveal very strong anisotropy in oxygen bandwidth leading to a reversal of the $e_g$ crystal field hierarchy. This work further establishes that the Mn atoms are sitting in a bath of a uniaxial exchange field that gradually goes out-of-plane to in-plane as the Mn doping level is increased. Overall, the behavior has some similarities with Mn doped GaAs and may be relevant to the physics of dilute magnetic semiconductors.

\textsuperscript{1}ALS Doctoral Fellowship, Advanced Light Source, LBNL.

10:12AM X31.00010 Temperature dependence of a zero bias anomaly in scanning tunnelling spectra of Sr(4)Ru(3)O(10)\textsuperscript{1} , BERNHARD NANSSEU, TATJANA NOVGORODOV, MICHAEL WAELSCHE, JÜRGEN HAGER, University of Kassel, JIANDI ZHANG, Florida International University, Miami, R. MOORE, WARD PLUMMER, Oak Ridge National Laboratory, ZHIQIANG MAO, Tulane University, RENE MATZDORF, University of Kassel — We have studied a zero bias anomaly in scanning tunnelling spectra of layered ruthenate Sr(4)Ru(3)O(10). This material shows a dip-like feature in the dI/dV spectra, which has previously observed in the single-layer Sr(2)RuO(4) and double-layer Sr(3)Ru(2)O(7) ruthenates. We have studied in particular the temperature dependence of the zero bias anomaly, which is in all three materials different. The triple-layer material shows intergrowth of single and double layers, which have been identified by their spectroscopic fingerprint. Finally, we discuss different effects as possible explanations for the zero bias anomaly.

\textsuperscript{1}The work was supported by NSF-DMR0346826 and the Deutsche Forschungsgemeinschaft.

10:24AM X31.00011 Anisotropy of magneto resistivity in trilayered ruthenate Sr$_4$Ru$_3$O$_{10}$\textsuperscript{1} , Evidence for orbital dependent metamagnetism , D. FOBES, M. ZHOU, T.J. LIU, Z. QU, Tulane University, USA, H.Q. YUAN, M. SALAMON, University of Illinois, Urbana-Champaign, USA, Z.Q. MAO, Tulane University, USA — Trilayered ruthenate Sr$_4$Ru$_3$O$_{10}$ is ferromagnetic with $T_c \approx 100K$ and moderate in-plane magnetic field ($B_c \approx 2T$) induces an itinerant metamagnetic transition [1,2]. Such metamagnetism within a FM ground state cannot be understood with a single band model of a field-tuned Stoner transition. We have measured azimuthal angular dependence of in-plane and out-of-plane magneto resistivity ($\rho_{ab}(\phi)$ and $\rho_c(\phi,B)$). We found that for B$<$B$_{c}$, at fixed field $\rho_{ab}(\phi)$ exhibits a two-fold anisotropy attributable to anisotropic behavior of an Ising ferromagnet, while $\rho_c(\phi)$ does not show such a behavior. For B$>$B$_{c}$, both $\rho_{ab}(\phi)$ and $\rho_c(\phi)$ exhibit a four-fold symmetry anisotropy, but the minimum value in $\rho_{ab}(\phi)$ and $\rho_c(\phi)$ occurs along different directions, i.e., [100] and [010] for $\rho_{ab}$, and [110] and [110] for $\rho_c$. Such a difference in anisotropic behavior between $\rho_{ab}(\phi)$ and $\rho_c(\phi)$ provides strong support that metamagnetism in Sr$_4$Ru$_3$O$_{10}$ is orbital dependent, i.e., ferromagnetic and metamagnetic bands coexist.


Work at Tulane is supported by NSF, DOE and the Research Corporation.

10:36AM X31.00012 Fermi Surface mapping of Sr$_4$Ru$_3$O$_{10}$ using Angle Resolved Photoemission , R.S. SINGH, F. WANG, J.W. ALLEN, University of Michigan, J.D. DENLINGER, Lawrence Berkeley National Lab, X.N. LIN, GANG CAO, University of Kentucky — Layered strontium ruthenates in the Ruddlesden-Popper series (Sr$_{n+1}$Ru$_n$O$_{3n+1}$) are scientifically interesting and technologically promising materials exhibiting various novel electronic and magnetic properties. We will show the effect of dimensionality on the electronic structure as one goes from two dimensional to three dimensional crystal structures by increasing n. In particular, we will present new results and analysis of photon energy dependent angle resolved photoemission spectroscopy measurements on Sr$_4$Ru$_3$O$_{10}$ and make detailed comparison of Fermi surface maps with recently measured Shubnikov-de Haas frequencies and available LDA band structure calculations corresponding to various layered strontium ruthenates.

Work supported by U.S. DOE (DE-AC03-76SF00098 at ALS, DE-FG02-07ER46379 at UM currently) and U.S. NSF (DMR-03-02825 at UM initially, DMR-02-40813 at UK).
Studies of MTJ crystal structure have implications for the development of high-performance MTJs, making them viable for MRAM and sensor applications. Careful engineering of the MgO tunnel barriers, CoFeB electrodes, and their interfaces is essential for high levels of tunneling magnetoresistance (TMR), particularly the CoFeB/MgO/CoFeB system, which exhibits large TMR. Unfortunately, these magnetoresistance devices suffer from considerable noise.

Incorporating a very desirable trait for magnetic random access memory and hard drive read heads, theory predicts high levels of tunneling magnetoresistance (TMR) which are achievable with magnetic tunnel junctions (MTJs) featuring the necessary elements for picoTesla MTJ sensors. However, challenges such as high noise levels and the need for greater precision in the performance of such MTJs exist in the integration of the necessary components of the sensor and illustrate the trade-offs that must be considered. For example, values of the TMR above 100% contribute very little, while lowering the saturation field of the free layer below 10 Oe is essential. These and other insights identify the critical issues than need attention and can guide research into productive directions.

We investigated MTJs with rf-sputtered or electron-beam evaporated MgO barrier layers, and we used TaN, Ta/Ru, and Ta/CuN as alternative seed layers for the MTJ growth. We report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.

We have studied the complex longitudinal ($\sigma_{xx}$) and transverse ($\sigma_{xy}$) conductivities in a series of Ca$_x$Sr$_{1-x}$Ru$_2$O$_3$ films by using the Landau-Lifshitz-Gilbert equation in non-linear regime. The results also suggest that this new experimental technique to detect FMR is very useful for characterizing the LA-FMR. Using the same structure, we electrically detected the LA-FMR of the Py by measuring the tunneling resistance in a sweeping external dc magnetic field. We will report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.

Using the same structure, we electrically detected the LA-FMR of the Py by measuring the tunneling resistance in a sweeping external dc magnetic field. We will report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.

1. Varying the anneal temperature, MgO growth methods, and seed layers, we have examined texturing in CoFeB/MgO/CoFeB tunnel junctions using x-ray diffraction. We investigated MTJs with rf-sputtered or electron-beam evaporated MgO barrier layers, and we used TaN, Ta/Ru, and Ta/CuN as alternative seed layers for the MTJ growth. We report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.


5. PHILIP PONG, ROBERT MCMICHAEL, NIST, EDMUND NOWAK, University of Delaware, ALAN EDELSTEIN, JAMES BURNETTE, GREG FISHER, Army Research Lab — The extension of small, inexpensive, low-power, low-frequency, ultra-sensitive magnetic sensors to fields between 1 nanoTesla and 1 picoTesla, an area currently dominated by fluxgates, optically-pumped magnetometers, and SQUIDs, would be a paradigm shift for the field of magnetic sensors. The necessary elements for picoTesla MTJ sensors have been identified by modeling the noise characteristics. The results help identify the experimental challenges that exist in the integration of the necessary components of the sensor and illustrate the trade-offs that must be considered. For example, values of the TMR above 100% contribute very little, while lowering the saturation field of the free layer below 10 Oe is essential. These and other insights identify the critical issues than need attention and can guide research into productive directions.

8:00AM X32.00001 Challenges for picoTesla Magnetic-Tunnel-Junction Sensors

PHILIP PONG, ROBERT MCMICHAEL, NIST, EDMUND NOWAK, University of Delaware, ALAN EDELSTEIN, JAMES BURNETTE, GREG FISHER, Army Research Lab — The extension of small, inexpensive, low-power, low-frequency, ultra-sensitive magnetic sensors to fields between 1 nanoTesla and 1 picoTesla, an area currently dominated by fluxgates, optically-pumped magnetometers, and SQUIDs, would be a paradigm shift for the field of magnetic sensors. The necessary elements for picoTesla MTJ sensors have been identified by modeling the noise characteristics. The results help identify the experimental challenges that exist in the integration of the necessary components of the sensor and illustrate the trade-offs that must be considered. For example, values of the TMR above 100% contribute very little, while lowering the saturation field of the free layer below 10 Oe is essential. These and other insights identify the critical issues than need attention and can guide research into productive directions.

8:12AM X32.00002 X-Ray Diffraction Studies of CoFeB/MgO/CoFeB Magnetic Tunnel Junctions

PINSHANE HUANG, Carleton College. JOHN READ, ROBERT BUHRMAN, Cornell University — MgO-based magnetic tunnel junctions (MTJs) show high levels of tunneling magnetoresistance (TMR), a very desirable trait for magnetic random access memory and hard drive read heads. Because theory links tunnel junction crystallinity with high TMR, studies of MTJ crystal structure have implications for the development of high-performance MTJs. Varying the anneal temperature, MgO growth methods, and seed layers, we have examined texturing in CoFeB/MgO/CoFeB tunnel junctions using x-ray diffraction. We investigated MTJs with rf-sputtered or electron-beam evaporated MgO barrier layers, and we used TaN, Ta/Ru, and Ta/CuN as alternative seed layers for the MTJ growth. We report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.

8:24AM X32.00003 Chemical and electronic studies of CoFeB / MgO / CoFeB magnetic tunnel junctions

J. READ, J. CHA, Cornell University, P. HUANG, Carleton College, W. EDELHOFF, NIST, D. MULLER, R. BUHRMAN, Cornell University — MgO-based magnetic tunnel junctions (MTJs), particularly the CoFeB/MgO/CoFeB system, exhibit large tunneling magnetoresistance (TMR) which makes them viable for MRAM and sensor applications. Careful engineering of the MgO tunnel barriers, CoFeB electrodes, and their interfaces is essential for optimizing device performance. We have studied the complex longitudinal ($\sigma_{xx}$) and transverse ($\sigma_{xy}$) conductivities in a series of Ca$_x$Sr$_{1-x}$Ru$_2$O$_3$ films by using the Landau-Lifshitz-Gilbert equation in non-linear regime. The results also suggest that this new experimental technique to detect FMR is very useful for characterizing the LA-FMR. Using the same structure, we electrically detected the LA-FMR of the Py by measuring the tunneling resistance in a sweeping external dc magnetic field. We will report on changes in both tunnel barrier and electrode crystallization as a function of anneal temperature, which we find to be dependent on both the MgO deposition method and the seed layer composition. Our complete MTJ structures using rf-sputtered MgO barriers achieve TMR in excess of 200%, and correlation with these XRD results sheds light on the complex dependence of MTJ performance on growth and processing conditions.

8:36AM X32.00004 FMR spectroscopy with very large precession cone angle in magnetic tunnel junctions

TAKAHIRO MORIYAMA, XIN FAN, JOHN Q. XIAO, Department of Physics and Astronomy, University of Delaware — Unlike the small angle precession with low power microwave excitation, which has been extensively studied using conventional ferromagnetic resonance (FMR) techniques, the large angle precession involves nonlinear response of the magnetizations. Large angle ferromagnetic resonance (LA-FMR) measurements can help to understand the magnetization dynamics with high power excitation generally found in current induced spin switching and microwave assisted switching, etc. Recently we have performed magnetoresistance measurements in IrMn/FeCo/AIOx/Permalloy (Py) magnetic tunnel junctions excited by a large power microwave [1]. Using the same structure, we electrically detected the LA-FMR of the Py by measuring the tunneling resistance in a sweeping external dc magnetic field. We found that the resonance frequency depends on the microwave power, i.e. precession cone angle, as well as the dc magnetic field, which can be well explained by using the Landau-Lifshitz-Gilbert equation in non-linear regime. The results also show that this new experimental technique to detect FMR is very useful for characterizing the LA-FMR.

8:48AM X32.00005 Technique for Minimizing the Effect of 1/f Noise in Magnetic Sensors

ALAN EDELSTEIN, GREG FISCHER, JAMES BURNETTE, U.S. Army Research Laboratory, SHU-FAN CHENG, Naval Research Laboratory, EDMUND NOWAK, Dept. of Physics and Astronomy, Univ. of Delaware, Newark, DE, WILLIAM EDELHOFF, NIST, Gaithersburg MD, CATHY NORDMAN, NVE, Eden Prairie MN — Sensors such as magnetic tunnel junctions with MgO barriers offer the possibility of increased sensitivity. The magnetoresistance of these junctions can be as large a 400%. Unfortunately, these magnetoresistance devices suffer from having considerable 1/f noise. We have a device, the MEMS flux concentrator, that modulates the field at the position of the sensor and thus increase the frequency of the field to be detected to kHz frequencies where the 1/f noise is much smaller. It does this by having flux concentrators on MEMS flaps that are driven to move electrostatic comb drives. The flaps on each side of the sensor are connected by springs so that the desired motion is a normal mode. The signal appears as sidebands that can be demodulated using a lock-in amplifier. The device will increase the sensitivity at 1 Hz of many sensors by a factor of 100. Tests indicate that the device does not increase the noise and that it will function at frequencies lower than 1 Hz. Results of initial tests will be reported.
This approach is demonstrated using super-paramagnetic particles of 2 \( \mu \)m. An optical tweezers was used to trap and position a single super-paramagnetic particle over a Spin Valve sensor, with the particle then detected by the sensor.

Using Spin Valve Sensors

The exchange bias increased at low temperatures from 50Oe to 350Oe when FeMn layers are on both surfaces of Co terminated [FeMn10nm/Co4nm/FeMn10nm] multilayer, compared to single FeMn layer. However for the Gd terminated [FeMn10nm/Co4nm/FeMn10nm] multilayer the Gd/FeMn interface does not induce exchange bias. Moreover exchange spring behavior is observed around compensation temperature due to the uncompensated moment in FeMn layers.

The work at UTA was supported by a grant No(Y-1215) from The Welch Foundation.

9:24AM X32.00008 Exchange bias in a ferrimagnetic/antiferromagnetic system\(^1\). M.R. HOSSU, The University of Texas at Arlington, Arlington, TX 76019, S. DEMIRTAS, M.B. SALAMON, University of Texas at Dallas, Richardson, TX 75083, A.R. KOYMEM, The University of Texas at Arlington, Arlington, TX 76019 — The effect of antiferromagnetic FeMn on ferrimagnetic (Co4nm/Gd4nm)\(_1\) multilayer was investigated by measuring the exchange bias and coercivity fields. It was observed that magnetic properties depend on whether the multilayers are Co or Gd terminated. The exchange bias increased at low temperatures from 500e to 3500e when FeMn layers are on both surfaces of Co terminated [FeMn10nm/Co4nm/FeMn10nm] multilayer, compared to single FeMn layer. However for the Gd terminated [FeMn10nm/Co4nm/FeMn10nm] multilayer the Gd/FeMn interface does not induce exchange bias. Moreover exchange spring behavior is observed around compensation temperature due to the uncompensated moment in FeMn layers.

\(^1\)The work at UTA was supported by a grant No(Y-1215) from The Welch Foundation.

10:36AM X32.00014 Interplay of Magnetic and Structural Anisotropy in CoNi Multilayer Thin Films . JOSEPH DVORAK, NSLS, BNL, KATHRYN KRYCKA, NCNR, NIST, JEAN-MARC BEAUJOUR, WENYU CHEN, ANDREW KENT, New York University, CHI-CHANG KAO, NSLS, BNL — Interfacial perpendicular magnetic anisotropy (PMA) is important for spin transfer devices and has been predicted to overcome dipolar shape anisotropy for [t Co|2t Ni] multilayers with thicknesses, t , of 4 Å or less [1]. Layered between Cu, however, thickness dependent PMA (t=1, 2, 3, 4 and 6 Å) is not sufficiently strong to produce perpendicular magnetization. Anomalous diffraction reveals that the Co and Ni are exponentially strained by the Cu within the sample plane. As calculated in reference 2 this trilgonal strain would be sufficient to overcome the PMA. Ferromagnetic resonance measurements [3] indicate that the net Lande g-factors are enhanced above bulk for all thicknesses, and increase further with decreasing layer thickness. By applying element-specific x-ray magnetic circular dichroism (XMCD) we have been able to study the Co and Ni individually. Both elements show increasing spin to orbit ratios with decreasing thickness magnetized either in-plane or along sample normal. In all cases the spin to orbit ratio is enhanced along the sample normal compared with the in-plane direction. [1] Phys. Rev. Lett. 68, 682 (1992) [2] Phys. Rev. B 69, 104424 (2004) [3] Eur. Phys. J. B 59, 475 (2007)

10:48AM X32.00015 Classical and Quantum Routes to Linear Magnetoresistance . JINGSHI HU, University of Chicago & Massachusetts Institute of Technology, T.F. ROSENBAUM, University of Chicago — We show that either adding a few parts per million of the proper chemical impurities to indium antimonide, a well-known semiconductor, or redesigning the material’s structure on the micrometer scale, can transform its response to an applied magnetic field. The former approach is a spectacular manifestation of magnetotransport in the extreme quantum limit, when only one Landau band is partially filled; the latter a classical outgrowth of disorder, turned to advantage. In both cases the magnetoresistive response at the heart of magnetic sensor technology can be converted to a simple, large and linear function of field that does not saturate. Harnessing the effects of disorder has the further advantage of extending the useful applications range of such a magnetic sensor to very high temperatures by circumventing the usual limitations imposed by phonon scattering.

Friday, March 14, 2008 8:00AM - 10:48AM
Session X33 MAGM FIAP DMP: Focus Session: Magnetic Resonance in Magnetic Semiconductors
Morial Convention Center 224


1Work supported by the NSF under project ECS-0608763.

8:12AM X33.00002 Spin Resolved Cyclotron Resonance and Magneto-absorption in InSb Multiple Quantum Wells1 . XINGYUAN PAN, G.D. SANDERS, C.J. STANTON, University of Florida, T. KASTURIARACHCHI, W. GEMPEL, X.H. ZHANG, R.C. MEYER, N. GOEL, M. EDIRISORIYA, T.D. MISHIMA, R.E. DOEZEMA, M.B. SANTOS, University of Oklahoma, Y.J. WANG, National Institute for Quantum and Complex Dynamics, University of California Santa Barbara — The nitrogen-vacancy (N-V) impurity center is a promising solid- state spin system for solid-state quantum information processing. Many desirable quantum properties have been found at room temperature, including long spin-coherence times, demonstration of single N-V spin quantum gate operation, discovery of rapid spin polarization and achievement of readout of single N-V spins. There have been many EPR experiments to investigate electronic structures and dynamics of impurities in diamond. Most of the studies were however performed by low-field EPR. High-frequency EPR generally has a great advantage for spectral and time resolution and absolute sensitivity due to very high spin-polarizations in high magnetic fields. High-frequency EPR for the diamond system therefore enables the investigation of ensembles of low-concentration impurities. In this presentation, we will discuss high-field properties of spin relaxations of impurities on diamond studied with 240 GHz cw and pulsed EPR.

1NSF DMR-0510056, DMR-0520550 and OISE-0530220.

8:24AM X33.00003 High-frequency EPR of impurities on diamond . SUSSUMU TAKAHASHI, MARK S. SHERWIN, Institute for Quantum and Complex Dynamics, University of California Santa Barbara, RONALD HANSON, DAVID D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California Santa Barbara — The nitrogen-vacancy (N-V) impurity center is a promising solid- state spin system for solid-state quantum information processing. Many desirable quantum properties have been found at room temperature, including long spin-coherence times, demonstration of single N-V spin quantum gate operation, discovery of rapid spin polarization and achievement of readout of single N-V spins. There have been many EPR experiments to investigate electronic structures and dynamics of impurities in diamond. Most of the studies were however performed by low-field EPR. High-frequency EPR generally has a great advantage for spectral and time resolution and absolute sensitivity due to very high spin-polarizations in high magnetic fields. High-frequency EPR for the diamond system therefore enables the investigation of ensembles of low-concentration impurities. In this presentation, we will discuss high-field properties of spin relaxations of impurities on diamond studied with 240 GHz cw and pulsed EPR.
8:36AM X33.00004 Electron-nuclear interactions in lightly-doped GaAs, studied through optically-detected magnetic resonance (ODMR)\(^1\). JOHN COLTON, Brigham Young University, LEE WIENKES, University of Minnesota-Twin Cities, ANDREW GIERKE, University of Wisconsin-Madison, SUSAN ALLEMANN, University of Wisconsin-La Crosse, ALLAN BRACKER, Naval Research Laboratory — Electron-nuclear interactions have been studied in lightly-doped GaAs via optically-detected magnetic resonance (ODMR). Thermally-polarized electrons were resonated with ~10 GHz microwaves; the spin states were detected with cw optical Kerr rotation. The electron-nuclear interaction was manifested through an effective magnetic field produced by the hyperfine interaction between nuclei and donor electrons, which caused a shift in the electron ODMR peak position. The effective nuclear field could be eliminated by simultaneous magnetic resonance of the three nuclear species. A measurement of the nuclear spin relaxation time was obtained (5.6 minutes) by tracking the amount of effective nuclear field, in the absence of nuclear magnetic resonance. Finally, optically-detected electron-nuclear double resonance (ODENDOR) was also performed, by monitoring changes in the electron Kerr rotation signal while sweeping through nuclear resonant frequencies one at a time.

\(^1\)Work supported by NSF, ACS/PRF, and Research Corporation

8:48AM X33.00005 Pseudospin Resonance in Semiconductor Bilayers, SAEED H. ABEDINPOUR, MARCO POLINI, MARIO P. TOSI, NEST-CNR-INFN and Scuola Normale Superiore, I-56126 Pisa, Italy, BILAL TANATAR, Department of Physics, Bilkent University, Bilkent, 06800 Ankara, Turkey, ALLAN H. MACDONALD, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri 65211, USA — The pseudospin degree of freedom in a semiconductor bilayer gives rise to a collective mode analogous to the ferromagnetic resonance mode of a ferromagnet. We present a theory of the dependence of the energy and the damping of this mode on layer separation \(d\). Based on these results, we discuss the possibility of realizing transport-current driven pseudospin-transfer oscillators in semiconductors.

9:00AM X33.00006 Location and Magnetic Hyperfine Properties of Mn\(^{2+}\) in Silicon, R.H. PINK, SUNY Albany, ARCHANA DUBEY, UCF Orlando, S.R. BADU, SUNY Albany, R.H. SCHEICHER, Upsalla University, Sweden, M.B. HUANG, SUNY Albany, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — Crystalline Silicon doped with the transition metal ion Mn\(^{2+}\) is ferromagnetic at room temperature and thus potentially a useful material for spintronic applications. In attempting to understand from first principles the location of Mn\(^{2+}\) and the electronic structure of the ferromagnetic system we have started work first on the dilute system. We have used the Hartree-Fock cluster procedure to determine the binding energies of the three likely locations for Mn\(^{2+}\), substitutional (S), tetrahedral interstitial (\(T_i\)) and hexagonal interstitial (\(H_i\)) locations allowing for relaxation of the silicon neighbors. Our calculations show that the H\(_i\) location is unstable and the S and \(T_i\) are stable. Our nuclear magnetic hyperfine interactions results for \(^{57}\)Mn nucleus and \(^{29}\)Si neighbor will be presented and compared with electron spin resonance \([1]\) experimental data.


9:12AM X33.00007 The Nuclear Spin Relaxation in the Semiconductor Double Quantum Dots: Study of Spin Diffusion, EDDY YUSUF, XUEDONG HU, Physics Department, University at Buffalo, SUNY, Buffalo 14260 — We study the relaxation of the nuclear spins in a semiconductor double quantum dot. We focus on spin diffusion as an important channel for nuclear spin relaxation. The diffusion of the nuclear spin polarization arises from the Fermi contact hyperfine interaction between electrons in the quantum dots and the nuclear spins, as well as the magnetic dipolar interaction between nuclear spins. We calculate the nuclear spin polarization relaxation time and the nuclear diffusion constant within the density matrix framework. We explore the behavior of the relaxation time and diffusion constant for a wide range of conditions, including variations in temperature, the initial degree of nuclear polarization, dot sizes, and the strength of the applied magnetic field. We compare our results to the available experimental data and discuss various experimental schemes to further test the outcome of our calculation. \([1]\) A. Greilich, et al., Science 317, 1896 (2007) \([2]\) S. Das Sarma, et. al., Solid State Commun. 133, 737 (2005)

9:24AM X33.00008 Microscopic theory of electron spin relaxation in N@C\(_{60}\), Z.G. YU, SRI International — Endohedral N@C\(_{60}\) exhibits an extremely long electron spin relaxation time and offers a great potential in storing and processing quantum information. Here we present a microscopic theory of electron spin relaxation in N@C\(_{60}\). The theory combines (1) the spin-orbit interaction of N 2p electrons, which mixes the ground state \(^4\)S with excited \(^2\)P and \(^2\)D states, and (2) the coupling between the N 2p electrons and C\(_{60}\) H\(_v\) vibrations, which facilitates transitions between \(^2\)P and \(^2\)D states. The spin relaxation occurs via a two-phonon (Raman) process by absorbing a H\(_v\) phonon and emitting another at the (approximately) same frequency. The theory consistently explains measured spin relaxation time \(T_1\) and its temperature dependence, and predicts two distinct spin decoherence \(T_2\) constants. In addition, the excellent agreement between theory and experiment suggests a universal importance of the two-phonon Raman process in determining spin relaxation in nanosstructures such as quantum dots, where a one-phonon process is ineffectual in flipping electron spins because of the lack of low-energy phonons in nanostuctures.

\(^3\)This work was supported by the Office of Basic Energy Sciences, Department of Energy.

9:36AM X33.00009 Electronic and transport properties of a lateral triple quantum dot molecule in a magnetic field, F. DELGADO\(^1\), Y.-P. SHIM, M. KORKUSINSKI, P. HAWRYLAK, Quantum Theory Group, Institute for Microstructural Sciences, NRC, Ottawa, ON, Canada K1A 0R6 — We present a theory of spin, electronic and transport properties of a few-electron lateral triangular triple quantum dot molecule in a magnetic field. Our theory is based on a Hubbard model and the Linear Combination of Harmonic Orbitals combined with Configuration Interaction method to arbitrary magnetic fields. The one-particle spectra obtained as a function of the magnetic field exhibit Aharonov-Bohm oscillations. As a result, by changing the magnetic field it is possible to engineer the degeneracies of single-particle levels, and thus control the total spin of the many-electron system. For the triple dot with two and four electrons we find oscillations of total spin due to the singlet-triplet transitions occurring periodically in the magnetic field. In the three-electron system we find a transition from a magnetically frustrated to the spin-polarized state. The impact of these phase transitions on the addition spectrum are analyzed and the qualitative behaviour of the current through the quantum molecule under spin blockade conditions is studied as a function of the applied magnetic field.

\(^1\)Department of Physics, University of Ottawa, MacDonald Hall, 150 Louis Pasteur, Ottawa, ON, Canada KIN 6N5
to previous Si(100) studies, we observe three resonant peaks, which we attribute to a) the two well known hyperfine spilt phosphorus resonances, and b) the of phosphorus donor electrons in silicon. These studies have been undertaken on the Si (100) interface, due to its wide utilization in the semiconductor industry.

CHRISTOPH BOEHME, Department of Physics, University of Utah — Recently, there has been a large effort towards the electrically detection of spin coherence manipulation in high fields, and these results will also be discussed.

microscopic processes leading to the signals discussed. Finally, pulsed EDMR (Rabi oscillations, Hahn echos) was performed to investigate spin coherence and defects near the Si-SiO₂ interface, were observed. The temperature dependence of the observed signals in the range T = 3K - 10K will be presented, and the microscopic processes leading to the signals discussed. Finally, pulsed EDMR (Rabi oscillations, Hahn echos) was performed to investigate spin coherence and manipulation in high fields, and these results will also be discussed.

10:12AM X33.00012 Electrically-detected magnetic resonance in accumulation-layer MOSFETs, LAURENS WILLEM VAN BEVEREN, University of New South Wales, DANE MCCAMEY, University of Utah, HANS HUEBL, Technische Universität München, ANDREW FERGUSON, University of Cambridge, TIM DUTY, ROBERT CLARK, University of New South Wales — Spin-dependent transport, originating from neutral-impurity scattering, in silicon accumulation-layer MOSFETs was reported more than a decade ago in an electron-spin resonance (ESR) cavity setup [1]. There, current measurements on the MOSFET showed ESR features with a hyperfine (HF) splitting of 42 G, indicative of electrons whose wavefunctions overlap with phosphorous nuclei in the silicon crystal. Here, we report the observation of electrically-detected magnetic resonance (EDMR) in phosphorus-doped silicon MOSFETs without the constraint of a cavity and down to the mK-regime in a dilution refrigerator with a superconducting magnet.

Instead, the ESR-field is generated by an on-chip shorted coplanar stripline (CPS), allowing broadband operation. Continuous-wave EDMR was achieved up to 30 GHz. The EDMR spectra show (i) the two hyperfine-split (42 G) ESR lines and (ii) an EDMR signal that is centered between the hyperfine lines, associated with the ‘free electron’ ESR response. [1] R. Ghosh and W. Silsbee, Phys. Lett. 85, 439 (1992).

10:24AM X33.00013 Electrically detected magnetic resonance in Si:P at high magnetic fields (B = 8.5 T), DANE MCCAMEY, Department of Physics, University of Utah, GAVIN MORLEY, London Centre for Nanotechnology, LOUIS CLAUDE BRUNEL, JOHAN VAN TOL, National High Magnetic Field Laboratory, Florida State University, HEATHER SEIPEL, CHRISTOPH BOEHME, Department of Physics, University of Utah — Phosphorus doped silicon (Si:P) is a technologically important material with possible uses in spintronic and quantum information processing devices. A useful way to understand the properties of this material is by investigation of the spin dependence of its transport processes. Whilst numerous studies of this type have been performed on Si:P at low magnetic fields, no systematic investigation has been undertaken at high magnetic fields. We will present an electrically detected magnetic resonance (EDMR) study of Si:P, with a native oxide surface, at B = 8.5 T (f_{resonance} ~ 240 GHz). The change in the sample photocurrent, ΔI/I, was measured as a function of B using a microwave chopping method. Resonant signals from the P donors, as well as P₁ defects near the Si-SiO₂ interface, were observed. The temperature dependence of the observed signals in the range T = 3 K - 10 K will be presented, and the microscopic processes leading to the signals discussed. Finally, pulsed EDMR (Rabi oscillations, Hahn echos) was performed to investigate spin coherence and manipulation in high fields, and these results will also be discussed.

10:36AM X33.00014 Pulsed electrically detected magnetic resonance of phosphorus donors near the Si(111)-SiO₂ interface, SEOYOUNG PAIK, HEATHER SEIPEL, SANG-YUN LEE, THOMAS HERRING, DANE MCCAMEY, CHRISTOPH BOEHME, Department of Physics, University of Utah — Recently, there has been a large effort towards the electrically detection of spin coherence of phosphorus donor electrons in silicon. These studies have been undertaken on the Si (100) interface, due to its wide utilization in the semiconductor industry. Here, we present a pulsed electrically detected magnetic resonance study on P donors near the Si(111) interface. We observe the transient current after a short, coherent microwave pulse as a function of both the magnitude and relative orientation (with respect to the [111] direction) of the applied magnetic field. Similar to previous Si(100) studies, we observe three resonant peaks, which we attribute to a) the two well known hyperfine split phosphorus resonances, and b) the P₁f defect resonance. The P₁f resonance exhibited an anisotropy with field direction, in agreement with conventional ESR studies. In addition, we observe a fourth isotropic resonance, with a g-factor of g = 2.0051±0.0004. We conclude that, aside from the anticipated and well known P-P₁ transition, at least one additional spin dependent recombination pathway exists at the Si(111)-SiO₂ interface.
8:12AM X35.00002 “Ultimate” SOI MOSFETs

THOMAS J. WALLS, KONSTANTIN K. LIKHAREV, Stony Brook University

— Silicon-On-Insulator (SOI) field-effect transistors (MOSFETs) are being aggressively scaled toward the 10-nm frontier - see, e.g., Ref. [2]. In our earlier work [1], we have carried out a detailed analysis of the performance and parameter variation sensitivity of double-gate sub-10-nm MOSFETs using a self-consistent numerical solution of the 2D Poisson equation and 1D Schrodinger equation. However, for very small devices the 1D approximation misses some important details of the device physics. In this work, we have used the momentum-space formalism, developed in 1989 by A. Szafer and A. D. Stone [3] to fully account for 2D quantum effects.

At the meeting, we will present a comparison of our new results with our previous 1D approximation, as well as calculations of the gate capacitance of the transistors. This work has been supported in part by the ONR.


8:24AM X35.00003 Novel Ferroelectric CMOS Nonvolatile Logic

M. TAKAHASHI, T. HORIUCHI, Q.-H. LI, S. WANG, K. Y. YUN, S. SAKAI, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — We propose a novel and promising nonvolatile-logic circuit constructed by p channel type (Pch) and n channel type (Nch) ferroelectric gate field effect transistors (FeFETs), which we named a ferroelectric CMOS (FeCMOS) circuit. The circuit works as both logic and memory. We fabricated a NOT logic FeCMOS device which have Pt metal gates and gate oxides of ferroelectric SrBi2Ta2O9 (SBT) and high-k HfAlO on Si. Key technology was adjusting threshold voltages of the FeFETs as well as preparing those of high quality. We demonstrate basic operations of the NOT-logic response, memory writing, holding and non-destructive reading. The memory writing is done by amplifying the input node voltage to a higher level when the node was logically high and to a lower one when it was logically low just before the writing operation. The data retention was also measured. The retained high and low voltages were almost unchanged for 1.2 days. The idea of this FeCMOS will enhance flexibility of circuit designing by merging logic and memory functions. This work was partially supported by NEDO.

8:36AM X35.00004 Study on threshold voltages of Pt/SrBi2Ta2O9/Hf-Al-O/Si FeFETs

Q.-H. LI, M. TAKAHASHI, S. WANG, T. HORIUCHI, C.C. WANG, K.Y. YUN, Y. FUHIHATA, S. SAKAI, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan — Complementary ferroelectric-gate field-effect transistors (FeFETs) are attractive for nonvolatile-logic circuit applications after the achievement of long data retention for both n- and p-channel FeFETs [1, 2]. To demonstrate nonvolatile logic circuits, the threshold voltage should be well controlled. Due to ferroelectricity two threshold voltages $V_{t,\text{left}}$ and $V_{t,\text{right}}$ can be defined from $I_d = V_{ds}$ curves as gate voltages at $I_d = 10^{-6}$ A. More than 90 n- or p-channel Pt/SrBi2Ta2O9/Hf-Al-O/Si FeFETs on a Si chip are studied. The average $V_{t,\text{left}}$ and $V_{t,\text{right}}$ are 1.19 and 2.38 V for n-channel FeFETs, and -0.76 and 0.40 V for p-channel FeFETs, respectively. The standard deviations of $V_t$ are 3-5% and 7-8% of the memory window for the n- and p-channel FeFETs, respectively. $V_t$ positions are adjusted by varying the well doping concentrations. Our results indicate possible circuit demonstration. This work was partially supported by NEDO.


8:48AM X35.00005 The Nanowire iJFET

BART SOORE, WIM MAGNUS, IMEC, Kapeldreef 75, B-3001 Leuven, Belgium — The cylindrical geometry of nanowire surrounding gate MOSFETs gives rise to outstanding electrostatic control in comparison to planar devices. On the other hand, we expect that for ultrasmall nanowire diameters, the interaction of electrons with the surface (e.g. surface roughness and high-k) will be detrimental for device performance due to mobility degradation. In order to avoid these surface interactions we consider a surrounding nanowire operated not in MOSFET mode, but in “JFET mode.” We thus consider a nanowire with silicon body radius $R$ and surrounding oxide of thickness $t_{ox}$ with a surrounding metal gate where both source, drain and silicon body are doped uniformly with a donor density $N_D$. Applying a negative gate voltage pushes the electrons away from the interface between the insulator and metal gate, and as a result a depletion region is induced. For sufficient negative gate voltage the depletion region reaches the center of the silicon body, and pinch-off occurs. For large radii, we construct a compact model, and we show that reasonable pinch-off voltages are realized when the wire radius or the donor density is sufficiently small. Using the gradual channel approximation we are able to obtain current-voltage characteristics that constitute a “proof of concept” for this device. In the case of ultrasmall radii, we perform a quantum mechanical analysis of the electronic structure.

9:00AM X35.00006 Extraordinary Electroconductance in Ti-GaAs hybrid thin film structures

YUN WANG, A.K.M. NEWAZ, JIAN WU, S.A. SOLIN, Washington University in St. Louis, V.R. KAVASSERI, NIU JIN, I.S. AHMAD, I. ADESIDA, University of Illinois at Urbana-Champaign — Device performance due to mobility degradation. In order to avoid these surface interactions we consider a surrounding nanowire operated not in MOSFET mode, but in “JFET mode.” We thus consider a nanowire with silicon body radius $R$ and surrounding oxide of thickness $t_{ox}$ with a surrounding metal gate where both source, drain and silicon body are doped uniformly with a donor density $N_D$. Applying a negative gate voltage pushes the electrons away from the interface between the insulator and metal gate, and as a result a depletion region is induced. For sufficient negative gate voltage the depletion region reaches the center of the silicon body, and pinch-off occurs. For large radii, we construct a compact model, and we show that reasonable pinch-off voltages are realized when the wire radius or the donor density is sufficiently small. Using the gradual channel approximation we are able to obtain current-voltage characteristics that constitute a “proof of concept” for this device. In the case of ultrasmall radii, we perform a quantum mechanical analysis of the electronic structure.

9:12AM X35.00007 Optimizing Transport Properties of a Potential Molecular Electronic Device

JULIO L. PALMA, CHAO CAO, HAI-PING CHENG, JEFFREY L. KRAUSE, University of Florida — Future generations of electronic devices will have the dimensions of molecular size. The ability to control the transport properties of single molecules will have a major impact on this promising technology. The azobenzene molecule has been proposed recently as a component of a light-driven molecular switch. This molecule has two stable conformations in its ground state: cis and trans. The molecule can be converted from one configuration to the other by photo-excitation. Previous calculations showed that the trans configuration has a considerably higher conductance than the cis configuration. In this work, we study the effects of chemical substituents on the electron transport properties of azobenzene. The effects of such substituents are crucial in predicting structures that may have optimized properties with slightly different chemical structures. For the azobenzene studies, we include electron donating groups (-NH2) and electron withdrawing groups (-NO2) in meta- and otho positions with respect the azo group. The transport properties are calculated using first principles methods that combine non-equilibrium Green’s function (NEGF) technique with density functional theory (DFT).

1DOE contract DE-FG02-02ER45995 to HP and JLK
9:24AM X35.00008 Ion Sources for Deep and Shallow Ion Implantation1 — ADY HERSHCOWITCH, BNL, V. BATALIN, I. TEP, A. BUGAEV, HCEI, V. GUSHENETS, B. JOHNSON, A. KOLOMIETS, G. KROPACHEV, R. KIBEBA, T. KULEVOY, I. LITOVKO, E. MASUNOV, E. OKS, V. PERSHIN, S. PETRENKO, S. POLOZOV, H. POOLE, PVI, OXARD CA, I. RUDSKOY, D. SELEZNEV, P. STOROZHENKO, A. SVAROVSKI, G. YUSHKOV — Various ions, but mostly B, P, Sb, & As, are implanted, over a wide range of energies into materials used in the construction of semiconductors. These energies range from as low as 100 eV for shallow surface implantations, to as high as multi-MeV for deep implantation into the substrate.

State of the art ion sources meet industry needs for the energy range of 10 eV to 300 keV. But at the two extremes (100’s of eV and at multi-MeV), there is room for improvement due to space charge limitations at the low energy range and due to inefficiency in acceleration at the higher energy range. A joint R&D effort focusing on meeting industry needs has been in progress for the past four years. This endeavor has resulted in record steady state output currents of higher charge state Antimony and Phosphorous ions as well as Decaborane molecular ions. This talk is a synopsis of an extensive ion source R&D program designed to address industry needs.

1Supported by DOE Contract No. DE-AC02-98CH1-886.

9:36AM X35.00009 Infrared Near-field Microscopy of Semiconductor Devices — FRITZ KEILMANN, ANDY J. HUBER, RAINER HILLEBRAND, Max-Planck-Institut für Biochemie — We report optical imaging at ultrahigh resolution < 30 nm of cross-sectional preparations of state-of-the-art transistors. Our technique employs a scanning optical near-field microscope of scattering type (s-SNOM). It is based on a tapping-mode AFM with a standard, metallized tip, and an interferometric receiver. This detects a pseudo-heterodyne signal detection that is filtered at a low harmonic of the tapping frequency. The illumination wavelength of 10.7 µm allows to record specific contrasts—which are obtained in amplitude as well as in phase—distinguishing not only all material components in the transistors, but furthermore highlighting the charge carriers. Prospects of quantitative carrier density mapping will be discussed. A.J. Huber et al., Adv. Mat. 19, 2209 (2007)

9:48AM X35.00010 Resistance Switching Behavior in Epitaxially Grown NiO — S.R. LEE, J.H. BAK, Y.D. PARK, K. CHAR, Seoul National University, D.C. KIM, R. JUNG, S. SEO, X.S. LI, G.S. PARK, I.K. YOO, Samsung Advanced Institute of Technology — Reproducible resistance switching behavior has been found in NiO films prepared by a pulsed laser deposition system. The I-V measurements of epitaxially grown NiO on SrRuO₃ electrode show a bipolar resistive memory switching behavior, in contrast with a unipolar switching behavior of polycrystalline NiO on Pt electrode. In order to understand the resistive memory switching mechanism in NiO, the I-V characteristics and memory switching property of epitaxial NiO prepared under various synthesis conditions and electrodes has been investigated. The IV measurements at room temperature suggest that the interface between NiO and the electrode plays an important role on the resistive switching phenomena. To analyze the role of the interface, our efforts to control the interfaces and to measure the I-V characteristics at low temperature will be presented.

10:00AM X35.00011 Temperature-Dependence of the Resonant Pump Wavelength in Optical Pumping Injection Cavity Lasers — L.J. OLAFSEN, Baylor University, K.G. YOUNG, University of Houston, T.C. MCALPINE, College of Wooster, W.W. BEWLEY, I. VURGAFTMAN, J.R. MEYER, U.S. Naval Research Laboratory, H. LEE, R.U. MARTINELLI, Sarnoff Corporation — An optical pumping injection cavity (OPIC) laser contains a type-II W active region enclosed between two GaSb/AlAsSb distributed Bragg reflector mirrors, where the thickness of the etalon cavity surrounded by the mirrors is tuned to the desired pump wavelength. Multiple reflections of the pump photons result in more efficient absorption of the pump beam and consequently higher efficiencies and lower lasing thresholds. An optical parametric oscillator is used to pump the OPIC lasers at resonance, where the threshold pump intensities are minimized and output efficiencies are maximized. The resonant pump wavelength varies linearly with temperature. In addition to presenting light-light results, including efficiencies and thresholds as a function of temperature, the temperature-dependence of the resonant pump wavelength will be discussed, including the relative variations and contributions of lattice constant and refractive index with temperature.

10:12AM X35.00012 Mid-IR Photonic-Crystal Interband Cascade Lasers — MUJIN KIM, CHUL SOO KIM, WILLIAM BEWLEY, CHADWICK CANEDY, JAMES LINDLE, JILL NOLDE, DIANE LARRABEE, IGOR VURGAFTMAN, JERRY MEYER, Code 5613, Naval Research Laboratory, Washington DC 20375, CODE 5613 NRL TEAM — Photonic-crystal distributed-feedback (PCDFB) semiconductor lasers have the potential to maintain optical coherence over very large areas. We report an electrically pumped PCDFB laser operating in a true single mode in the mid-infrared. A two-dimensional grating aperture was formed on top of an interband cascade laser emitting at 3.3 µm by patterning a high-index Ge layer. The grating and the 400-µm-wide gain stripe were tilted by 20° with respect to the facet. Current spreading was prevented by ion bombarding the region outside the gain stripe rather than etching of a ridge. The gain region at the edge of the cavity was terminated by ion bombardment, since feedback from the back facet is undesirable. A single mode was emitted with maximum cw output power > 60 mW, resolution-limited spectral linewidth (side-mode suppression ratio 27 dB), and single-lobe spatial far-field with angular full width at half maximum of 0.5°. Comparison of the near and far field patterns indicated effective $M^2 \approx 3$. The observation of low efficiency is thought to be due primarily to inadequate grating coupling, which can be remedied by thickening the Ge layer.

10:24AM X35.00013 ABSTRACT WITHDRAWN —

10:36AM X35.00014 Electrical Characterization of Critical Phase Change Conditions in Nanoscale Ge$_2$Sb$_2$Te$_5$ Pillars — OZKAN OZATAY, BARRY STIPE, JORDAN KATINE, BRUCE TERRIS, Hitachi Global Storage Technologies, San Jose Research Center, San Jose, CA 95135 — Following the original work of Ovshinsky on disordered semiconductors that exhibit ovonic threshold switching (OTS) there has been substantial interest in the electronic reversible switching properties of chalcogenides. The current induced phase transitions between amorphous and crystalline phases in these materials of magnitude changes in the electrical conductance which makes them an ideal candidate for non-volatile data storage applications. In this work we investigate the scaling of critical programming conditions required to observe such transitions between highly resistive (disordered) and highly conductive (ordered) states by constructing a resistance map with various pulse widths and amplitudes under different non-volatile data storage applications. In this work we investigate the scaling of critical programming conditions required to observe such transitions between highly resistive (disordered) and highly conductive (ordered) states by constructing a resistance map with various pulse widths and amplitudes under different non-volatile data storage applications. In this work we investigate the scaling of critical programming conditions required to observe such transitions between highly resistive (disordered) and highly conductive (ordered) states by constructing a resistance map with various pulse widths and amplitudes under different non-volatile data storage applications. In this work we investigate the scaling of critical programming conditions required to observe such transitions between highly resistive (disordered) and highly conductive (ordered) states by constructing a resistance map with various pulse widths and amplitudes under different non-volatile data storage applications.


10:48AM X35.00015 Charge Transport Phenomena in Detectors of the Cryogenic Dark Matter Search — KYLE SUNDQUIST, University of California, Berkeley, CDMS COLLABORATION — The Cryogenic Dark Matter Search (CDMS) seeks to detect putative weakly-interacting massive particles (WIMPS), which could explain the dark matter problem in cosmology and particle physics. By simultaneously measuring the number of charge carriers and the energy in athermal phonons created by particle interactions in intrinsic Ge and Si crystals at a temperature of 40 mK, a signature response for each event is produced. This response, combined with phonon pulse-shape information, allows CDMS to actively discriminate candidate WIMP interactions with nuclei apart from electromagnetic radioactive background which interacts with electrons. The challenges associated with these techniques are unique. Carrier drift-field are maintained at only a few V/cm, else drift-emitted Luke-Neganov phonons would dominate the phonons of the original interaction. Under such conditions, carrier scattering is dominated by zero-point fluctuations of the lattice ions. It has been an open question how well the 8 Kelvin data prominent in the literature depicts this case. We compare the simulated transport properties of electrons and holes in $< 100$ $\text{Ge}$ at 40 mK and at 8 K, and apply this understanding to our detectors.
Newton, Abbe, and the relation between refractive index and dispersion.

WILLIAM KARSTENS, Saint Michael’s College, DAVID Y. SMITH, University of Vermont and Argonne National Laboratory — Chromatic aberration in lenses is corrected by combining glasses with different index/dispersion characteristics. The correction is based on an empirical linear relation between index and dispersion, a rule known qualitatively for many years that was given definitive form by Abbe and Schott in 1886. Despite a long history, its physical basis has remained obscure. Here we show it is a consequence of the spectral shape of the glasses’ UV absorption by expanding the Kramers-Kronig relation for the index in a series of absorption-spectrum moments. To first order, the index is determined by the inverse-first moment, the dispersion by the inverse-third moment. For a complex glass, these moments may be rewritten as sums of UV-absorption moments for the glass-former and the glass-modifiers. The total index is then a series of absorption-spectrum moments. To first order, the index is determined by the inverse-first moment, the dispersion by the inverse-third moment. Newton’s erroneous conclusion that achromatic lenses could not be made was based on the limited range of glasses available to him, all of which fell on a single index-dispersion line.

8:12AM X36.00002 A Non-Perturbative Series Solution for Diffraction Gratings with Arbitrary Profiles

DANIEL NKEMZI, University of Buea, Cameroon, PRABASAJ PAUL, Denison University — In this work, we use a boundary continuation technique to obtain an iterative series expansion for the scattering of a plane wave by a diffraction grating with an arbitrary profile function. The method is efficient and is simple to apply. The results of numerical experiments show excellent agreement with the C-method and the coupled-wave approach.

8:24AM X36.00003 Surface-enhanced Raman scattering by silver clusters at planar dielectric interface above the critical angle.

DENIS PRISTINSKI, NIST, SILIYU TAN, HENRY DU, Stevens Inst of Tech — Light refraction at the planar interface of dielectric media prevents light propagation in the optically denser medium at angles above the critical value. This limitation is broken when the evanescent wave is excited at the opposite side of the interface. The polarization and angle dependence of the light emitted above the critical angle has been previously studied for both luminescence and elastic scattering. In this work we demonstrate the possibility to quantitatively characterize the effect using surface-enhanced Raman signal from thiocyanate molecules adsorbed on clustered silver nanoparticles at the water-glass interface. Evanescently excited silver nanoparticles demonstrate strong polarization dependence for both absorption and emission, and wider range of emission angles, as compared with the model of a radiating dipole at a similar interface.

8:36AM X36.00004 A novel time resolved resonance Raman technique - applications in correlated systems.

B. SCHULZ, I. MAHNS, A. GOOS, P. SAICHU, S. BINDER, S.G. SINGER, A. RUSYDI, M. RUEBHAUSEN, Institute of Applied Physics, University of Hamburg, D-20355 Hamburg, Germany, S.-W. CHEONG, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, P. GUPTASARMA, Department of Physics, University of Wisconsin, Milwaukee, Wisconsin 53211, USA — In many modern materials the functionality of a system can be observed by studying the order parameters in the time domain. Here, we present a time resolved pump probe resonance Raman system that allows to study order parameters in an energy range from 5 meV to several eV and in a time domain from 1 ps to several ns. Due to our fully achromat, all reflective Raman spectrometer, [1] we are able to combine pump and probe beams ranging in energy from the near infrared to the deep ultraviolet. We show exemplary measurements on the melting process in charge order Manganites (La₀.₆Ca₀.₄MnO₃) as well as studies on the temporal evolution of the superconducting parameter in high-Tc cuprates.


8:48AM X36.00005 The Physics of Coherent Anti-Stokes Raman Spectroscopy.

LASZLO UJJ, Department of Physics, University of West Florida, Pensacola, FL 32514 — Coherent anti-Stokes Raman Spectroscopy (CARS) has been shown to be one of the most powerful experimental methodologies for obtaining vibrational information from both stable and transient molecular species. The general theoretical and experimental principles associated with CARS, together with specific examples of its applications to important molecular systems, are presented. A concise theoretical formalism of CARS, and its electronically resonant variant, is presented with an emphasis on points relevant to the interpretation of experimental spectra. The instrumental components required for obtaining typical CARS data are illustrated in a brief description of a picoseconds and a nanosecond experimental system used to record CARS spectra. The details of the design and operation of an all solid-state broadband nanosecond CARS system will be presented. Specific examples of picosecond CARS data are taken from measurements of stable and transient intermediates comprising the photoresponses of photoactive proteins.

Polarization sensitive CARS spectra taken with the nanosecond system are also presented. Finally, an overview of developments in this field to be anticipated is discussed. Reference: Laszlo Ujj and George H. Atkinson, Coherent Anti-Stokes Raman Spectroscopy, in Handbook of Vibrational Spectroscopy, John Wiley and Sons, Ltd., 2002.

9:00AM X36.00006 High quality optical and mechanical properties of a dispersive optomechanical device.

ANDREW JAYICH, BENJAMIN ZWICKL, CHENG YANG, JACK HARRIS, Yale University — We have characterized the optical and mechanical properties of a high finesse Fabry Perot cavity (F=17,000) dispersively coupled to a micromechanical SiN₄ membrane. The membrane’s fundamental and higher-order vibrational modes show quality factors above 10⁶ and a spectrum corresponding to a simple drumhead model. The optical cavity’s transverse and longitudinal spectrum is also in agreement with theory. We find that the cavity’s full transmission and reflection properties can be modeled quantitatively once the membrane’s small optical loss is accounted for. We will discuss the role of avoided crossings between higher-order optical modes in this system, particularly within the context of potential QND measurements of micromechanical devices.

9:12AM X36.00007 Using Multiple FROG Traces to Generate a Single High Dynamic Range Trace.

SEBASTIAN W. WINKLER, WILLIAM M. DENNIS, University of Georgia, Department Physics and Astronomy — Frequency resolved optical gating (FROG) is a powerful technique that has been used to characterize the complex electromagnetic field of ultrafast pulses for more than a decade. However, FROG relies on detector with a high dynamic range; at least 10⁶. If the detector’s dynamic range is insufficient, the FROG phase retrieval code will not work properly. We describe a method to generate a single FROG trace with high dynamic range from multiple FROG traces of the same pulse but using different integration times. We present successfully retrieved fields from data captured using a spectrometer that would otherwise have insufficient dynamic range for FROG trace acquisition.
9:24AM X36.00008 Theoretical Considerations for Surface Thermal Lensing Studies Using Polarized Light. MARSHALL THOMSEN, Eastern Michigan University — Surface Thermal Lensing (STL) is a well-established photothermal technique for locally probing the optical, thermal, and mechanical properties of a surface. A periodically chopped laser beam, the pump beam, irradicates a sample. A portion of the pump beam is absorbed by the sample and converted into thermal energy, resulting in a periodic local thermal expansion of the surface. A second, weaker and broader laser beam, the probe beam, is directed off-normal at the surface, covering the entire heated area. The result is a modulated diffraction pattern embedded in the reflected portion of the probe beam. The addition of polarizers both between the probe laser and the sample and between the sample and the detector opens up the possibility of gaining further information about the surface. In particular, the repeated flexing of the surface of a polymer sample may give rise to local rearrangement of polymer chains. The resulting asymmetry may be visible through a polarization analysis of STL signals.

9:36AM X36.00009 Intra-valence transitions for uncooled short wave infrared detection1. A.G. UNIL PERERA, S.G. MATSIKS, P.V.V. JAYAWEERA, Georgia State University, H.C. LIU, M. BUCHANAN, National Research Council Canada, GEORGIA STATE UNIVERSITY USA TEAM, NATIONAL RESEARCH COUNCIL CANADA TEAM — An infrared detector based on p-GaAs/AlGaAs heterojunction exhibiting response in the 2-5 µm range at room temperature is demonstrated. The basic principle of the detector utilizes inter-valence (heavy hole, light hole, and split-off hole) absorption of a highly p-doped GaAs layer (emitter). The dark current is limited by the work function at the interface between the highly doped emitter and the undoped AlxGa1-xAs barrier. The barrier height can be tailored by varying the Al fraction to obtained the desired operating temperature. The split-off energy of the material determines the split-off threshold and the band offset determines the free carrier threshold for the photo excited carriers. Detector performance can be controlled by varying these two thresholds. A device consisting of 30 periods of 3×1016 cm-3 p-doped GaAs emitter and Al0.57Ga0.43As barrier regions between two contact layers shows infrared detection up to 330 K with a peak responsivity of 1.4 A/W and D* of 2.6×109 Jones at 2.5 µm. Different materials should give rise to different wavelength threshold infrared detectors operating at high temperatures.

1Work supported by US NSF grant # ECS 05-53051.

9:48AM X36.00010 Room Temperature Terahertz Detection based on Electron Plasma Resonance in an Antenna-Coupled Gallium Arsenide MESFET. SANGWOO KIM, Phys. Dept., UCSB, JERAMY ZIMMERMAN, Materials Dept., UCSB, PAOLO FOCARDI, Jet Propulsion Lab, Pasadena, CA, DONG HO WU, Naval Research Lab, Washington, D.C., ARTHUR C. GOSSARD, Materials Dept., UCSB, MARK S. SHERWIN, Phys. Dept., UCSB — Terahertz detectors utilizing quantum transitions require cryogens since the thermal energy (kT) needs to be smaller than the transition energy (1 THz ~ 4 meV). A bulk 3-D plasma is a classical excitation, and hence does not saturate with temperature. Plasma absorptions occur at a density-dependent frequency 1/2π√(n_DAD2/me). For 1 THz radiation, the corresponding 3-D free electron density is n_D ~ 1015 cm-3 in GaAs, a density that can be easily achieved. The density of electrons can be made tunable if a device such as a Field Effect Transistor is employed. We utilize these facts in order to realize a room temperature Terahertz detector. Our device consists of twin-slot antennas, coplanar waveguides, and a GaAs Metal-Semiconductor-Field-Effect-Transistor (MESFET). While the sensitivity of the first set of devices is not competitive, we were able to observe the resonance behavior by sweeping bias voltages. This talk will present design, fabrication, recent measurement, and possible future improvement of our detector. Work supported by NSF-DMR 0703925 and Naval Research Lab.

10:00AM X36.00011 Signal Restoration from Atmospheric Degradation in Terahertz Spectroscopy. DONG HO WU, Naval Research Laboratory, SEONG KONG, Temple University — We present a method of restoring signals in Terahertz (THz) spectroscopy by removing the distortion from the observed THz signals. The distortion is generated by the absorption and scattering of gas molecules and water vapor in the atmosphere, during the transmission of THz beams through the air from the source to the spectrometer. Such atmospheric degradation causes spurious spectral dips and peaks in the THz spectrum, which often obscure the spectral peaks specific to the material of interest. This fact makes it challenging to measure the THz spectroscopic signatures of objects at a distance in a humid air environment. A THz signal restoration filter based on an artificial neural network model can be very effective in removing noisy absorption peaks caused by atmospheric degradation in THz spectra.

10:12AM X36.00012 Compressed Sensing and its Applications in Imaging. DHARMPAL TAKHAR, TING SUN, JASON LASKA, MARCO DUARTE, RICHARD BARANIUK, KEVIN KELLY, Department of Electrical and Computer Engineering, Rice University, Houston, Texas — Compressed sensing is a new sampling theory which allows reconstructing signals using sub-Nyquist measurements/sampling. This can significantly reduce the computation required for image/video acquisition/encoding, at least at the sensor end. Compressed sensing works on the concept of sparsity of the signal in some known domain, which is incoherent with the measurement domain. We exploit this technique to build a single pixel camera based on an optical modulator and a single photosensor. Random projections of the signal (image) are taken by optical modulator, which has random matrix displayed on it, corresponding to the measurement domain (random noise). This randomly projected signal is collected on the photosensor and later used for reconstructing the signal. In this scheme we are making a tradeoff between the spatial extent of sampling array and a sequential sampling over time with a single detector. In addition to this method, we will also demonstrate a new design which overcomes this shortcoming by parallel collection of many random projections simultaneously. Applications of this technique in hyperspectral and infrared imaging will be discussed.

10:24AM X36.00013 Test of search methods to extract quasi-periodical signals in noise from gravitational wave detectors. GIOVANNI SANTOSTASI, McNeese State University — We have tested several techniques to extract quasi-periodical signals in a simulated advanced gravitational wave detector noise. These methods include chi-square, Zn-square, H-test and Bayesian methods. The efficiency and usefulness, in different contexts, of these methods is discussed.

10:36AM X36.00014 High temperature resonant ultrasonic spectroscopy methods. GUANGYAN LI, University of Mississippi, GARY LAMBERTON, General Electric Corporation, JOSH GLADDEN, University of Mississippi — Resonant ultrasonic spectroscopy (RUS) is a technique to obtain the full elastic tensor of single crystal materials by measuring the mechanical resonances of a polished sample. Any direct resonance measurement at high temperatures is limited by the fact that most ultrasonic transducers have an upper operational limit of 200-300°C. High temperature RUS measurements are made possible by separating the sample, placed in a tube furnace, and the transducers with buffer rods made of low acoustic attenuation materials with good thermal stability such as ceramic alumina or fused quartz. Tests on stainless steel demonstrated that the system has the ability of acquiring resonance signals at temperatures up to 800°C. Experimental issues such as additional resonance peaks introduced by the buffer rods and sample loading will be addressed. The apparatus has been used to study high temperature elastic properties of p-zint, piezoelectrics, single crystal quartz, a novel piezoelectric material kepertite, and the glass transition around 400°C in bulk metallic glass compounds. Good results from these studies and high temperature test runs of aluminum and stainless steel demonstrate the potential for RUS measurements at elevated temperatures.
10:48AM X36.00015 Development of a low cost, low temperature cryocooler using the Gifford McMahon cycle. A. RAMANAYAKA, R. MANI, Georgia State University — Although Helium is the second most abundant element, its concentration in the earth’s atmosphere is fairly low and constant, as the portion that escapes from the atmosphere is replace by new emission. Historically, Helium was extracted as a byproduct of natural gas production, and stored in gas fields in a National Helium Reserve, in an attempt to conserve this interesting element. National policy has changed and the cost of liquid Helium has increased rapidly in the recent past. These new circumstances have created new interest in alternative eco-friendly methods to realizing and maintaining low temperatures in the laboratory. There have been number of successful attempts at making low temperature closed cycle Helium refrigerators by modifying an existing closed cycle system, and usually the regenerator has been replaced in order to achieve the desired results. Here, we discuss our attempt to fabricate a low cost, low temperature closed cycle Helium refrigerator starting from a 15K Gifford McMahon system. We reexamine the barriers to realizing lower temperature here and our attempts at overcoming them.

Friday, March 14, 2008 8:00AM - 10:48AM
Session X37 FIAP: Semiconductors IV: Electronic and Optical Properties II Morial Convention Center

8:00AM X37.00001 Electronic Structure of Silicon Phases Resulting from Decompression from $\beta$-Sn1, BRAD MALONE, JAY SAU, MARVIN COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We present an ab initio study of the electronic structure of the silicon phases that result from decompression from the metallic $\beta$-Sn phase, namely the BC8 (Si III), the hexagonal diamond (Si IV), the R8 (Si XII), and the yet unobserved ST12 phases. To correct for the inadequacies in the DFT-LDA quasiparticle energy spectra we employ quasiparticle corrections with the framework of the GW approximation. In doing so we find that the R8 phase should be semiconducting at lower pressures We also analyze the effect of strain and doping on these materials in an attempt to find novel applications for these phases, from high-mobility semiconductors to superconductivity.

1This work was supported by the National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and NPACI

8:12AM X37.00002 First principles calculations of optical and x-ray spectra from atomic coordinates alone1, J.J. KAS, M. PRANGE, F.D. VILA, Y. TAKIMOTO, J.J. REHR, University of Washington — Theoretical calculations of various x-ray and optical spectroscopies often rely on semi-empirical or phenomenological models to account for many-body effects and thermal vibrations. Typically such models include a number of parameters which complicate fitting schemes that extract physical quantities from experimental spectra. Here we present an approach for ab initio calculations of these spectra starting from structure alone. A many-pole model of the dielectric function is introduced to calculate the self-energy and spectral function[2] while a density functional theory calculation of the dynamical matrix is used to calculate effects of thermal vibrations. [2] In addition, core-hole effects are incorporated with RPA screening. [2] This approach has been incorporated into FEFF9, a new version of the real-space multiple-scattering FEFF code for broad spectrum calculations of various optical and x-ray spectra.

1Supported by DOE Grant DE-FG02-97ER45623 (JIR and MP), NIH NCRR BTP grant RR-01290 (JK), NSF 0120967 (YT).


8:24AM X37.00003 Surface states of the Topological Insulator Bi$_{1-x}$Sb$_x$. JEFFREY TEO, LIANG FU, CHARLES KANE, University of Pennsylvania — The alloy Bi$_{1-x}$Sb$_x$ is a narrow gap semiconductor for .07 < x < .22. Based on the bulk bandstructures of Bi and Sb this material was recently predicted to be a three dimensional strong topological insulator (STI). The STI is distinguished from ordinary insulators by a $Z_2$ topological invariant characterizing the bulk and by the presence of topologically protected surface states, whose Fermi arc encloses an odd number of Dirac point. Here we study the surface states of the 111 face of Bi$_{1-x}$Sb$_x$ using a semi infinite tight binding model. This calculation demonstrates explicitly the topological character of the surface states. In addition, we examine other robust, model independent features of the surface states which arise due to (1) charge neutrality at the surface, (2) the presence in the bulk bandstructure of a 3 dimensional Dirac point with a small mass and (3) the presence of mirror symmetry, which leads to an additional topological characterization of the band structure in terms of a mirror Chern integer. Implications for photoemission experiments will be discussed.

1 NSF grants DMR-0605066

8:36AM X37.00004 Optical, Electronic and Structural Properties of Y$_x$Sc$_{1-x}$N. ROBERT BRUCE VANDOVER, JOHN GREGOIRE, STEVE KIRBY, Cornell University — Semiconducting Y$_x$Sc$_{1-x}$N thin films are reactively sputtered onto a variety of surfaces, resulting in films varying from nanocrystalline to epitaxial (single crystalline). As a function of composition, we investigate the variations in the crystalline lattice, Hall mobility, absorptivity and direct and indirect band gaps. We find this material to be a solid solution semiconductor across the entire composition range. The tunable band gap and high absorptivity of this semiconductor make it an interesting photovoltaic material. Details on this application will be presented as well as prospects of this material’s use as the host for ferromagnetic transition metals.

8:48AM X37.00005 Free-electron induced mode mixing and surface-polariton enhanced reflected THz-field. DANHONG HUANG, USAF Research Lab, GODFREY GUMBS, Hunter College of CUNY, PLAU ALSING, DAVE CARDIMONA, USAF Research Lab — The main result of this talk is the prediction of large enhancements at the band edges of a coupled Bloch-surface-plasmon-polariton band in the spectrum of the reflected far electromagnetic field due to anti-crossing gaps induced by the strong coupling between the continuous surface-plasmon-polariton mode and the discrete Bloch-like modes. The existence of these Bloch-like modes is a direct consequence of the nonlocal mixing of specular and diffraction modes of the reflected electromagnetic field by free-electron induced optical polarization and the interference of a pair of surface optical-polarization waves with opposite Bragg order numbers in the presence of a grating. The interference of these two counter-propagating surface waves leads to the formation of a Wannier-like state with associated electromagnetic fields localized within the grating-gap regions. The effects of the sheet density, grating period and absorption loss on the optical enhancements of both transmitted and reflected electromagnetic fields are investigated.
9:00AM X37.00006 Absorption and Photoluminescence Analysis of InAs/GaSb Superlattices Exhibiting Lateral Composition Modulation. JULIA WICKETT, University of Houston, JIANHUA LI, Rigaku Americas Corp., DONNA STOKES, University of Houston — The effects of lateral composition modulation (LCM) in (InAs)$_{1/2}$/(GaSb)$_{1/2}$ superlattices on the structure and optical response of the material have been investigated by double crystal x-ray diffraction (XRD). infrared absorption and photoluminescence (PL). Superlattices (SL) grown by molecular beam epitaxy (MBE) on GaSb (001) substrates with InSb interfacial bonds. Various buffer/substrate combinations were employed to determine if strain manipulation could be used to improve the optical response of the system. Modeling of XRD data has been used to determine the strain state of the SL layers with respect to the growth template. Absorption and PL measurements indicate that strain significantly affects the optical responses of the samples and manipulation and control over the strain state of the system will be key in employing LCM superlattices for optical applications.

9:12AM X37.00007 Probing ErAs nanoparticle density of states using capacitance-voltage$^1$, KASEY RUSSELL, VENKATESH NARAYANAMURTI, Harvard University, JOSHUA ZIDE, ARTHUR GOSSARD. UC Santa Barbara — Two asymmetric In$_{0.53}$Ga$_{0.47}$As/In$_{0.53}$Al$_{0.47}$As double-barrier samples are fabricated and compared using low-temperature capacitance-voltage measurements. The two samples are identical except for a layer of ErAs nanoparticles embedded within the quantum well layer of one of the samples. A clear difference in the capacitance-voltage profile is observed between the two samples, and the difference is attributed to additional available states associated with the ErAs nanoparticles. These results are compared with a charge-step simulation of the low-frequency capacitance of the device in order to estimate the density of states contributed by the ErAs nanoparticles.

1Supported by the Office of Naval Research through ONR/MURI and NSF/NNIN through use of Harvard’s Center for Nanoscale Systems.

9:24AM X37.00008 Photon-like plasmon polariton in a nanocoaxial waveguide$^1$, YUN PENG, XIWEN WANG, KRZYSZTOF KEMPFA, Boston College — We study propagation of electromagnetic waves in a nano-coaxial waveguide for frequencies below the surface plasmon frequency. We show, that for sufficiently low frequencies, the waveguide supports a photon plasmon mode that resembles, and indeed reduces to the conventional TEM mode of the conventional coaxial, known in the radiotechnology. We consider also coupling of the mode to the external radiation, and show that it can be made very efficient with appropriate antenna-like arrangements.

1Supported in part by grants from MITTc and Solasta Inc.

9:36AM X37.00009 X-ray Absorption Study of Amorphous Metal Semiconductor Alloys $M_xS_i_{1-x}$ (M: Gd, Y) Near the Metal Insulator Transition. ERIK HELGREN, F. HELLMAN, UC Berkeley, LI ZENG, UCSD, J.W. FREELAND, P. RYAN, D. HASKEI, R. WINARSKI, Argonne National Lab, M. VAN VEENENDAAL, N. Illinois University, R. WU, UC Irvine — X-ray absorption structure (XAS) at both Si K edges and Gd M edges were measured at compositions close to the metal insulator transition (MIT) for amorphous $Gd_xS_i_{1-x}$ ($x = 0.11 - 0.21$) and $Y_xS_i_{1-x}$ ($x=0.13$) from 10-300K. Spectral lineshape is unchanged as a function of composition, despite the presence of the MIT at $x = 0.14$. Comparison with calculations indicates that Gd is in the $3+$ state for all compositions and temperatures measured. An anomalous temperature dependence of the MIT is observed, and we provide a theoretical explanation for this behavior. Based on this result we offer an alternative explanation for the MIT, which is related to charge transfer or $4f$ charge transfer or $4f$-edge resonant inelastic x-ray scattering (RIXS) experiment, we found that resonant enhancements occur both near and above the Eu L$_3$ absorption peak. In both resonance experiments, we identify a number of narrow energy loss features and compare those features with the optical spectroscopy spectrum. Interestingly, we observed a drastic dependence on measurement geometry in a resonant enhancement above the Eu L$_3$ absorption peak. We discuss the excitation symmetry based on the geometry dependence. This study demonstrates the utility of the rare-earth L$_3$-edge RIXS as a probe of excited states in rare-earth systems.

1Supported in part by NIST Grant 70 NAMB 2H003 (APS) and DOE Grant DE-FG03-97ER45623 (JJR).

10:00AM X37.00011 Effect of Dielectric Response on the Magic Angle Mystery in EELS$^1$. ADAM SORINI, JOHN REHR, University of Washington, ZACHARY LEVINE, National Institute of Standards and Technology — The “magic” collection angle in electron energy-loss spectroscopy (EELS) is that angle at which the collection angle in an anisotropic sample “magically” becomes orientation independent. The “mystery” is that non-relativistic theory predicts a magic angle typically a factor of two too large in modern EELS experiments. Recently it has been shown that a relativistic treatment largely explains the discrepancy [1]. Here, we suggest that the dielectric response of the sample can lead to still larger angle corrections for low-energy-loss spectra [2]. These dielectric effects are included in a relativistic, independent particle theory using the generalized Lorentz gauge. The effect is illustrated by a calculation of the magic angle including both relativistic and first principles dielectric corrections for graphite and for boron nitride.


1Supported in part by NIST Grant 70 NAMB 2H003 (APS) and DOE Grant DE-FG03-97ER45623 (JJR).

10:12AM X37.00012 Wave-front engineering by Huygens-Fresnel principle for nonlinear optical interactions in domain engineered structures. ZHU YONGYUAN, Nanjing University — The wave-front engineering for nonlinear optical interactions was discussed. Using Huygens-Fresnel principle we developed a general theory and technique for domain engineering with conventional quasi-phase-matching (QPM) structures being the special cases. We put forward the concept of local QPM, which suggests that the QPM is fulfilled only locally not globally. Experiments agreed well with the theoretical prediction. The proposed scheme integrates three optical functions: generating, focusing and beam splitting of second-harmonic wave, thus making the device more compact. This work was supported by the State Key Program for Basic Research of China (Grant No. 2004CB619003) and also by the NNSF of China (Grant Nos.10523001, 10504013 and 10674065).
10:24AM X37.00013 Influence of Phonon dimensionality on Electron Energy Relaxation1, ILARI MAASILTA, JENNI KARVONEN, University of Jyväskylä — We studied experimentally the role of phonon dimensionality on electron-phonon (e-p) interaction in thin copper wires evaporated either on suspended silicon nitride membranes or on bulk substrates, at sub-Kelvin temperatures. The power emitted from electrons to phonons was measured using sensitive normal metal-insulator-superconductor (NIS) tunnel junction thermometers. Membrane thicknesses ranging from 30 nm to 750 nm were used to clearly see the onset of the effects of two-dimensional (2D) phonon system. We observed for the first time that a 2D phonon spectrum clearly changes the temperature dependence and strength of the e-p scattering rate, with the interaction becoming stronger at the lowest temperatures below ∼ 0.5 K for the 30 nm membrane.1


10:36AM X37.00014 Hartree-Fock-Cluster Investigation of Nuclear Quadrapole Interactions in Solid Chalcogens, Selenium and Tellurium.1, M.M. ARYAL, Tribhuvan University, Nepal, N.B. MAHARJAN, Tribhuvan University Nepal, SUNY Albany, D.D. PAUDYAL, D.R. MISHRA, S.R. BYAHUT, Tribhuvan University, Nepal, R.H. SCHEICHER, Upsala University, Sweden, S.R. BADU, SUNY Albany, J. JEOG, Univ. Ulsan South Korea, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany, UCF Orlando — Using the first-principles Hartree-Fock-Cluster Procedure, we have studied the electronic structures of pure chain like Selenium and Tellurium, pure ring structured Selenium, Tellurium impurity in chain and ring-structured Selenium and Tellurium impurity in chain-structured Tellurium chain. For our investigations in all the systems we have carried out convergence studies with respect to variational basis set sizes, sizes of clusters and electron correlation effects using many-body perturbation theory. Using our calculated electronic field-gradient parameters q in the pure chain systems and employing the experimental quadrupole coupling constants (e2Q), the values Q(77Se)=(0.50±0.04) × 10−28 m2 and Q(125Te)=(0.2 ±0.2) × 10−28 m2. Results will also be presented for the asymmetry parameters η for the pure chain systems and the e2Q and η for 77Se in selenium ring. Our calculated values for e2Q and η for the impurity systems will also be presented and compared with available experimental data and earlier theoretical results.

Friday, March 14, 2008 8:00AM - 10:24AM —
Session X39 GSNP: Miscellaneous Topics in Statistical Physics Mortional Convention Center 231

8:00AM X39.00001 Enhancement of epidemic extinction by random vaccination1, IRA SCHWARTZ, Naval Research Laboratory, MARK DYKMAN, Michigan State University — We study the probability of epidemic extinction in large populations. We use the susceptible-infected-susceptible (SIS) model since it forms the foundation of many epidemic processes. Fluctuations in the SIS system have two sources. The major source is the randomness of the “reactions” in which the number of susceptibles and/or infected changes. In addition, we assume that vaccination is done at random, leading to the decrease of the number of susceptibles. The vaccination is modeled by a Poisson process. The probability distribution is found from the master equation, which is solved in the eikonal approximation. It is shown that, even in the absence of vaccination, the logarithm of the extinction rate displays scaling dependence on the parameters. It scales as the square of the distance to the parameter value where the average number of infected vanishes. This is very different from the familiar 3/2 scaling law for saddle-node bifurcations. Finally, we show that even weak vaccination can dramatically increase the extinction probability. The correction to the logarithm of the probability becomes exponential in the vaccination rate when this rate is not too small.

1 Research supported by the Office of Naval Research and Army Research Office

8:12AM X39.00002 Inhomogeneous Coupling in 2-Channel Asymmetric Simple Exclusion Processes, KONSTANTINOS TSEKOURAS, ANATOLY KOLOMEISKY, Rice University — Asymmetric exclusion processes for particles moving on parallel channels with inhomogeneous coupling are investigated theoretically. Particles interact with hard-core exclusion and move in the same direction on both lattices, while transitions between the channels is allowed at one specific location in the bulk of the system. An approximate theoretical approach describing the dynamics in the vertical link and horizontal lattice segments exactly but neglecting the correlation between horizontal and vertical transport is developed. It allows us to calculate stationary phase diagrams, particle currents and densities for symmetric and asymmetric transitions between the channels. It is shown that in the case of the symmetric coupling there are three stationary phases, similarly to the case of single-channel totally asymmetric exclusion processes with local inhomogeneity. However, the asymmetric coupling between the lattices lead to a very complex phase diagram with ten stationary-state regimes. Extensive Monte Carlo computer simulations generally support theoretical predictions, although simulated stationary-state properties slightly deviate from calculated in the mean-field approximation, suggesting the importance of correlations in the system. Dynamic properties and phase diagrams are discussed by analyzing constraints on the particle currents across the channels.

8:24AM X39.00003 Brownian Gas: a field theory with a Poissonian ground state1, ANDREA VELENICH, CLAUDIO CHAMON, Physics Department, Boston University, DIRK KREIMER, Institut des Hautes Etudes Scientifiques and Department of Mathematics and Statistics, Boston University — As a first step towards a satisfying field theory of Brownian particles in interaction, we study exactly the non-interacting case, its combinatorics and its non-linear time-reversal symmetry. The field theory is nevertheless interacting; the vertex is the hallmark of the original particle nature of the gas and enforces the constraint of a strictly positive density field as opposed to a Gaussian free field. We compute exactly all the non-interacting case, its combinatorics and its non-linear time-reversal symmetry. The field theory is nevertheless interacting: the vertex is the hallmark of the

1 NSF Grant: DMS/0603781

8:36AM X39.00004 Wave electrophoretic trapping and chaos1, BOYD EDWARDS, LLOYD CARROLL, AARON TIMPERMAN, JARROD SCHIFFBAUER, JON MEASE, West Virginia University — Synchronized oscillating electric potentials are applied to a periodic array of stationary cylindrical electrodes in a stationary conducting viscous fluid. These potentials produce a longitudinal traveling wave that traps high-mobility ions that reveal the formation of intrinsic localized modes (ILMs) in a nonlinear electrical lattice. The lattice studied is a discrete transmission line consisting of two inductors and a diode (with voltage-dependent capacitance) per unit cell, and it forms a ring. We show that when this ring circuit is driven uniformly at large amplitudes, an instability of the uniform mode leads to the appearance of sharply localized features. Under certain driving conditions, these ILMs can become locked to the driver.

8:48AM X39.00005 Experimental Study of Energy Localization in a Nonlinear Electrical Lattice, LARS ENGLISH, RITOBAN BASU THAKUR, RYAN STEARRETT, DICKINSON COLLEGE, PHYSICS TEAM — Experimental results are presented that reveal the formation of intrinsic localized modes (ILMs) in a nonlinear electrical lattice. The lattice studied is a discrete transmission line consisting of two inductors and a diode (with voltage-dependent capacitance) per unit cell, and it forms a ring. We show that when this ring circuit is driven uniformly at large amplitudes, an instability of the uniform mode leads to the appearance of sharply localized features. Under certain driving conditions, these ILMs can become locked to the driver.
9:00AM X39.00006 Multiple traveling solitons in one-dimensional monatomic quartic lattices, SANGHAMITRA NEOGI, GERALD MAHAN. Department of Physics, The Pennsylvania State University — We discuss the generation of traveling soliton waves in a one-dimensional monatomic quartic lattice using numerical techniques. We apply an external forcing function or a pulse to the end atom of a free chain of monatomic atoms to generate traveling solitons. When the strength of the forcing function is above a threshold value, multiple traveling solitons are observed to flow down the chain. The number of traveling solitons in the chain increases rapidly with the increase in pulse strength beyond this critical value. The amplitudes and velocities of these multiple solitons increase with the increase in pulse strength for small pulse strengths. For larger values of pulse strengths, the amplitudes and velocities of all the multiple solitons saturate. The frequencies and wave vectors of all the traveling solitons on the quartic lattice are within a very narrow range of values. These values are independent of the pulse strength.

1Graduate Student
2Professor of Physics

9:12AM X39.00007 Statistical mechanics rooted in maximum entropy method shows absence of the Gibbs paradox, CHIH-YUAN TSENG, National Central University — Studying the Gibbs paradox problem indicates Gibbs's statistical mechanics may not be a general theory for thermodynamics. We found that most of conventional resolutions only provide explanations for “supplementary” introduction of the Gibbs correction rather than re-develop statistical theory to comprehend corresponding aspects. In this talk, we will show a general theory of statistical mechanics based on generalized maximum entropy method, which is designed for inductive inference. The general theory integrates prior knowledge of the system and measurements of macroscopic properties into a general ensemble. Based on the general theory, the 1/N! is simply a prior distribution that denotes our prior knowledge for indistinguishability of N microstates instead of the correction for the canonical ensemble. There is no Gibbs paradox. It is simply a consequence of incomplete statistical description for classical thermodynamic systems.

9:24AM X39.00008 High-Precision Thermodynamic and Critical Properties from Tensor Renormalization-Group Flows, MICHAEL HINCZEWSKI, TUBITAK - Bosphorus Univ., Feza Gursel Institute, A. NIHAT BERKER, Koç Univ., and M.I.T. — The recently developed tensor renormalization-group (TRG) method [1] provides a highly precise technique for deriving thermodynamic and critical properties of lattice Hamiltonians. The TRG is a local coarse-graining transformation, with the elements of the tensor at each lattice site playing the part of the interactions that undergo the renormalization-group flows. These tensor flows are directly related [2] to the phase diagram structure of the infinite system, with each phase flowing to a distinct surface of fixed points. Fixed-point analysis and summation along the flows give the critical exponents, as well as thermodynamic functions along the entire temperature range. Thus, for the ferromagnetic triangular lattice Ising model, the free energy is calculated to better than 10^{-5} along the entire temperature range. Unlike previous position-space renormalization-group methods, the truncation (of the tensor index range D) in this general method converges under straightforward and systematic improvements. Our best results are easily obtained with D = 24, corresponding to 4624-dimensional renormalization-group flows. [1] M. Levin and C.P. Nave, Phys. Rev. Lett. 99, 120601 (2007). [2] M. Hinczewski and A.N. Berker, arXiv:0709.2803v1 [cond-mat.stat-mech], Phys. Rev. E, in press.

9:36AM X39.00009 Nucleation in a long-range repulsive model, KIPTON BARROS, WILLIAM KLEIN, Boston University. — We employ a model with long-range repulsive interactions to study nucleation from a fluid to a crystalline phase. The long-range interactions make the metastable fluid phase long lived. From our simulations we find a divergence of the susceptibility at the spinodal, as predicted by mean-field theory. We also observe nucleation events and verify that the nucleating droplets, when they occur, match the numerical saddle point solutions of the free energy functional. In one dimension, where Alexander-McTague type symmetry arguments cannot be satisfied, we find that nucleation does not occur and that the fluid-solid transition is continuous. In two and three dimensions the transition is first order, with nucleating droplets of hexagonal and bcc symmetries.

1Supported in part by the NSF Grant No. DGE-0221680.

9:48AM X39.00010 Phase transitions in the long-range antiferromagnetic Ising model, RACHELE DOMINGUEZ, KIPTON BARROS, WILLIAM KLEIN, Boston University — We study the long-range antiferromagnetic Ising model to understand microphase separation in block-copolymer systems and dipolar Ising models. When quenched to low temperatures, the system initially obeys a Cahn-Hilliard-Cook-like linear theory and then orders into a "striped" or "clumpy" phase. The system also exhibits order-to-order transitions between the stable stripe and clump phases. From the free energy density obtained from coarse graining the Ising model, we use Langevin dynamics to investigate these transitions. I will discuss the nature of the transitions into the ordered phases as well as computational and theoretical methods for obtaining the phase diagram of the system.

10:00AM X39.00011 Emergent Structures in Dissipative Wave-Particle Systems, DAVIT SIVIL, ALFRED HUBLER, Center for Complex Systems Research, Department of Physics, University of Illinois at Urbana-Champaign — We study the motion of a particle with mass m on a vibrated string of length L. We assume that there is a friction force between the particle and the string. The string is sinusoidally forced at both ends. We find that the particle has attractors located at x=L/2 +/- nωc/2ω, where ω is the frequency of the waves on the string, and n ∈ Z. We also study the attractors of the same system with multiple driving frequencies. We also compared our results with numerical simulations.

10:12AM X39.00012 Absence of structural glass transition in a monoatomic model liquid predicted to undergo an ideal glass transition, MATTHIAS TROYER, CHARLOTTE GILS, HELMUT KATZGRABER, ETH Zurich — We study numerically a monodisperse model of interacting classical particles predicted to exhibit a static liquid-glass transition. Using a dynamical Monte Carlo method we show that the model does not freeze into a glassy phase at low temperatures. Instead, depending on the choice of the hard-core radius ends. We find that the particle has attractors located at x=L/2 - nπc/ω, where ω is the frequency of the waves on the string, and n ∈ Z. We also study the attractors of the same system with multiple driving frequencies. We also compared our results with numerical simulations.

Friday, March 14, 2008 8:00AM - 11:00AM — Session X40 DBP: Self Assembled Protein Cages Morial Convention Center 232

8:00AM X40.00001 A minimal model for protein coat dynamics in intracellular vesicular transport, RANJAN MUKHOPADHYAY, Clark University, HUI WANG, Lehigh University, GREG HUBER, University of Connecticut Health Center — Within eukaryotic cells, proteins are transported by vesicles formed from coated regions of membranes. The assembly of coat proteins deforms the membrane patch and drives vesicle formation. Once the vesicle has pinched off, the protein coat rapidly disassembles. Motivated by recent experimental results, we propose a minimal model for the dynamics of coat assembly and disassembly and study the spatio-temporal behavior of the system. We will show that for a range of parameters, our model can robustly generate a steady state distribution of protein clusters with characteristic sizes and will obtain the scaling behavior of average cluster size with the parameters of the model. We will also discuss the coupling of coat dynamics to sorting of cargo proteins.
8:12AM X40.00002 The study of viral assembly with fluorescence fluctuation spectroscopy . JOACHIM MUELLER, BIN WU, YAN CHEN, University of Minnesota — Enveloped viruses contain an encapsulating membrane that the virus acquires from the host cell during the budding process. The presence of the enveloping lipid membrane complicates the physical characterization of the proteins assembled within the virus considerably. Here we present a method based on fluorescence fluctuations that quantifies the copy number of proteins within an enveloped viral particle. We choose the viral protein Gag of the human immunodeficiency virus (HIV) type 1 as a model system, because Gag expressed in cells is sufficient to produce viral-like particles (VLPs) of the same size as authentic virions. VLPs harvested from cells that express fluorescently labeled Gag were investigated by two-photon fluorescence fluctuation spectroscopy. The autocorrelation functions of the fluctuations revealed a hydrodynamic size of the fluorescent VLPs consistent with previous results based on electron microscopy. Further analysis of the fluctuations revealed a copy number of Gag per virion that is inconsistent with the prevailing model of HIV assembly. We will discuss the implications of our experimental results for the assembly process of VLPs.

8:24AM X40.00003 Spherical Proteins and Viral Capsids Studied by Theory of Elasticity . ZHENGYANG YANG, Department of Physics & Astronomy, University of Pittsburgh, IVET BAHAR, Department of Computational Biology, University of Pittsburgh, MICHAEL WIDOM, Department of Physics, Carnegie Mellon University — Coarse-grained elastic network models have been successful in elucidating the fluctuation dynamics of proteins around their native conformations. It is well established that the low-frequency collective modes derived by simplified normal mode analysis depend on the overall 3-dimensional shape of the biomolecule. Given that the large scale collective motions are usually involved in biological function, our objective in this work is to gain more insights into large scale collective motions of spherical proteins and virus capsids by considering a continuous model with perfect spherical symmetry. To this end, we compare the global dynamics of proteins and the analytical solutions from an elastic wave equation with spherical boundary conditions. In addition, an icosahedral discrete model is generated and analyzed for validating our continuous model. Applications to lumazine synthase, satellite tobacco mosaic virus and other viruses shows that the spherical elastic model can efficiently provide insights on collective motions that are otherwise obtained by detailed elastic network models.

8:36AM X40.00004 Low frequency mechanical modes of viruses with atomic detail . ERIC DYKEMAN, OTTO SANKEY, Arizona State University — The low frequency mechanical modes of viruses can provide important insights into the large global motions that a virus may exhibit. Recently it has been proposed that these large global motions may be excited using impulsive stimulated Raman scattering producing permanent damage to the virus. In order to understand the coupling of external probes to the capsid, vibrational modes with atomic detail are essential. The standard approach to find the atomic modes of a molecule with \( N \) atoms requires the formation and diagonalization of a \( \sqrt{3N \times N} \) matrix. As viruses have \( 10^3 \) or more atoms, the standard approach is difficult. Using ideas from electronic structure theory, we have developed a method to construct the mechanical modes of large molecules such as viruses with atomic detail. Application to viruses such as the cowpea chlorotic mottle virus, satellite tobacco necrosis virus, and M13 bacteriophage show a fairly complicated picture of the mechanical modes.

8:48AM X40.00005 Diversity of in-vivo assembled HIV-1 capsids . SE IL LEE, TOAN NGUYEN, Physics, Georgia Institute of Technology — Understanding the capsid assembly process of Human Immunodeficiency Virus (HIV), the causative agent of Acute Immuno Deficiency Syndrome (AIDS), is very important because of recent intense interest in capsid-oriented viral therapy. The unique conical shapes of mature HIV-1 capsid have drawn significant interests in the biological community and started to attract attention from the physics community. Previous studies showed that in a free assembly process, the HIV-1 conical shape is not thermodynamically stable. However, if the volume of the capsid is constrained during assembly and the capsid protein shell has high spontaneous curvature, the conical shape is stable. In this work, we focus on in-vivo HIV-1 capsid assembly. For this case, the viral envelope membrane present during assembly imposes constraint on the length of the capsid. We use an elastic continuum shell theory to approximate the energies of various HIV-1 capsid shapes (spherical, cylindrical and conical). We show that for certain range of viral membrane diameter, the conical and cylindrical shapes are both thermodynamically stable. This result is supported by experimental observation that in-vivo assembled HIV-1 capsids are very heterogeneous in shapes and sizes. Numerical calculation is also performed to improve theoretical approximation.

9:00AM X40.00006 An elastic model of partial budding of retroviruses . RUI ZHANG, TOAN NGUYEN, School of Physics, Georgia Institute of Technology — Retroviruses are characterized by their unique infection strategy of reverse transcription, in which the genetic information flows from RNA back to DNA. The best known representative is the human immunodeficiency virus (HIV). Unlike budding of traditional enveloped viruses, retrovirus budding happens together with the formation of spherical virus capsids at the cell membrane. Led by this unique budding mechanism, we proposed an elastic model of retrovirus budding in this work. We found that if the lipid molecules of the membrane are supplied fast enough from the cell interior, the budding always proceeds to completion. In the opposite limit, there is an optimal size of partially budded virions. The zenith angle of these partially spherical capsids, \( \alpha \), is given by \( \alpha \sim (\tau^2/\kappa \sigma)^{1/4} \), where \( \kappa \) is the bending modulus of the membrane, \( \sigma \) is the surface tension of the membrane, and \( \tau \) characterizes the strength of capsid protein interaction. If \( \tau \) is large enough such that \( \alpha \approx \pi/2 \), the budding is complete. Our model explained many features of retrovirus partial budding observed in experiments.

9:12AM X40.00007 Calibrating elastic parameters from molecular dynamics simulations of capsid proteins . STEPHEN HICKS, CHRISTOPHER HENLEY, Cornell University — Virus capsids are modeled with elastic network models in which a handful of parameters determine transitions in assembly [1] and morphology [2]. We introduce an approach to compute these parameters from the microscopic structure of the proteins involved. We consider each protein as one or a few rigid bodies with very general interactions, which we parameterize by fitting the simulated equilibrium fluctuations (relative translations and rotations) of a pair of proteins (or fragments) to a 6-dimensional Gaussian. We can then compose these generalized springs into the global capsid structure to determine the continuum elastic parameters. We demonstrate our approach on HIV capsid protein and compare our results with the observed lattice structure (from cryo-EM [3] and AFM indentation studies).


9:24AM X40.00008 Coarse-grained mechanics of viral shells . WILLIAM S. KLUG, MELISSA M. GIBBONS, University of California, Los Angeles — We present an approach for creating three-dimensional finite element models of viral capsids from atomic-level structural data (X-ray or cryo-EM). The models capture heterogeneous geometric features and are used in conjunction with three-dimensional nonlinear continuum elasticity to simulate nanoindentation experiments as performed using atomic force microscopy. The method is extremely flexible; able to capture varying levels of detail in the three-dimensional structure. Nanoindentation simulations are presented for several viruses: Hepatitis B, CCMV, HK97, and \( \phi 29 \). In addition to purely continuum elastic models a multiscale technique is developed that combines finite-element kinematics with MD energetics such that large-scale deformations are facilitated by a reduction in degrees of freedom. Simulations of these capsid deformation experiments provide a testing ground for the techniques, as well as insight into the strength-determining mechanisms of capsid deformation. These methods can be extended as a framework for modeling other proteins and macromolecular structures in cell biology.

9:36AM X40.00009 ABSTRACT HAS BEEN MOVED TO SESSION C1 —
10:00AM X40.00011 Poisson pulsed control of particle escape\textsuperscript{1}, MARIE MCCRARY, LORA BILLINGS, Montclair State University, IRA SCHWARTZ, Naval Research Laboratory, Washington, DC, MARK DYKMAN, Michigan State University — We consider the problem of escape in a double well potential. With a weak background Gaussian noise, the escape rate is well known and follows an exponential scaling with the noise intensity $D$. Here, we consider adding a small Poisson noise to the Gaussian noise. We compute the change in escape time as we add Poisson distributed pulses of a given duration and amplitude. The escape rate acquires an extra factor which is determined by the system dynamics and is inversely proportional to $D$. As a result, for small $D$ even weak Poisson pulses can lead to a significant change of the escape rate. The Poisson noise induced factor depends sensitively on the interrelation between the noise correlation time and the relaxation time of the system. We compare analytical results with extensive numerical simulations. The numerical computation of escape rates for multiple interacting particles in a well will also be shown.

\textsuperscript{1}Research supported by the Army Research Office and the Office of Naval Research.

10:12AM X40.00012 Quorum sensing and biofilm formation investigated using laser-trapped bacterial arrays, VERNITA GORDON, JOHN BUTLER, IVAN SMALYUKH, MATTHEW PARSEK, GERARD WONG, University of Illinois, Urbana-Champaign — Studies of individual, free-swimming (planktonic) bacteria have yielded much information about their genetic and phenotypic characteristics and about “quorum sensing,” the autoinducing process by which bacteria detect high concentrations of other bacteria. However, in most environments the majority of bacteria are not in the planktonic form but are rather in biofilms, which are highly structured, dynamic communities of multiple bacteria that adhere to a surface and to each other using an extracellular polysaccharide matrix. Bacteria in biofilms are phenotypically very different from their genetically-identical planktonic counterparts. Among other characteristics, they are much more antibiotic-resistant and virulent. Such biofilms form persistent infections on medical implants and in the lungs of cystic fibrosis patients, where Pseudomonas aeruginosa biofilms are the leading cause of lung damage and, ultimately, death. To understand the importance of different extracellular materials, motility mechanisms, and quorum sensing for biofilm formation and stability, we use single-gene knockout mutants and an infrared laser trap to create a bacterial aggregate that serves as a model biofilm and allows us to measure the importance of these factors as a function of trapping time, surface, and nutritional environment.

10:24AM X40.00013 Self-Polarization of Cells in Elastic Gels, ASSAF ZEMEL, SAMUEL SAFRAN, Department of Materials and Interfaces, The Weizmann Institute of Science, Rehovot, 76100, Israel — The shape of a cell as well as the rigidity and geometry of its surroundings play an important role in vital cellular processes. The contractile activity of cells provides a generic means by which cells may sense and respond to mechanical features. The matrix stresses, that depend on the elasticity and geometry of cells, feedback on the cells and influence their activity. This suggests a mechanical mechanism by which cells control their shape and forces. We present a quantitative, mechanical model that predicts that cells in an elastic medium can self-polarize to form well ordered stress fibers. We focus on both single cells in a gel, as well as on an ensemble of cells that is confined to some region within the gel. While the magnitude of the cellular forces is found to increase monotonically with the matrix rigidity the anisotropy of the forces, and thus the ability of the cells to polarize, is predicted to depend non-monotonically on the medium’s rigidity. We discuss these results with experimental findings and with the observation of an optimal medium elasticity for cell function and differentiation.

10:36AM X40.00014 Active suspensions in shear flow\textsuperscript{1}, A. AHMADI, M.C. MARCHETTI, Physics Department, Syracuse University, Syracuse NY 13244, T.B. LIVERPOOL, Department of Mathematics, University of Bristol, Bristol BS8 1TW, UK — We report on the structure and rheology of an active suspension of cytoskeletal filaments and motor proteins in shear flow. Hydrodynamics equations for an active suspension were derived earlier by us [arXiv:q-bio.CB/0703029v1] by coarse-graining the Smoluchowski equation for a model of filaments and motors. The model incorporates the coupling of orientational order to flow and accounts for the exchange of momentum between filaments and solvent. In the present study we investigate the role of active crosslinkers on the formation and stability of ordered states (polar and nematic) under external shear flow. We also study the effect of motor activity on the rheological behavior of the ordered states away from boundaries. This work may also be relevant for the understanding of the flow-driven reorientation of endothelial cells under the shear stress imposed by blood flow.

\textsuperscript{1}This work was supported by the National Science Foundation through grant No. DMR-0705105.

10:48AM X40.00015 Selective advantage for sexual replication with random haploid fusion\textsuperscript{1}, EMMANUEL TANNENBAUM, Ben-Gurion University of the Negev — This talk develops a simplified set of models describing asexual and sexual replication in unicellular diploid organisms. The models assume organisms whose genomes consist of two chromosomes, where each chromosome is assumed to be functional if and only if it is equal to some master sequence. The fitness of an organism is determined by the number of functional chromosomes in its genome. For a population replicating sexually, a cell replicates both of its chromosomes and then divides and splits its genetic material evenly between the two cells. For a population replicating sexually, a given cell first divides into two haploids, which enter a haploid pool. Within the haploid pool, haploids fuse into diploids, which then divide via the normal mitotic process. When the cost for sex is small, as measured by the ratio of the characteristic haploid fusion time to the characteristic growth time, we find that sexual replication with random haploid fusion leads to a greater mean fitness for the population than a purely asexual strategy. The results of this talk are consistent with previous studies suggesting that sex is favored at intermediate mutation rates, for slowly replicating organisms, and at high population densities.

\textsuperscript{1}This research was supported by the Israel Science Foundation (Alon Fellowship) and by the United States - Israel Binational Science Foundation

11:15AM Y3.00001 Theoretical studies of quantum interference effects in graphene. EDWARD MCCANN, Lancaster University — We review the recently-developed theory of weak localization in monolayer and bilayer graphene [Phys. Rev. Lett. 97, 146805 (2006); Phys. Rev. Lett. 98, 176806 (2007)]. Owing to the chiral nature of electrons in a monolayer of graphite (graphene) one can expect weak antilocalization and a positive weak-field magnetoresistance in it. For high-density monolayer graphene and for any-density bilayers, the dominant factor affecting weak localization properties is trigonal warping of graphene bands, which reflects asymmetry of the carrier dispersion with respect to the center of the corresponding valley. The suppression of weak antilocalization by trigonal warping is accompanied by a similar effect caused by random-bond disorder (due to bending of a graphene sheet) and by dislocation/antidislocation pairs. As a result, weak localization in graphene can be observed only in samples with sufficiently strong inter-valley scattering due to atomically sharp scatterers or by edges in a narrow wire, reflected by a characteristic form of conventional negative magnetoresistance. We show this by evaluating the dependence of the magnetoresistance of graphene on relaxation rates associated with various possible ways of breaking a “hidden” valley symmetry of the system.

1 In collaboration with K. Kechedzhi, V.I. Falko, H. Suzuura, T. Ando, and B.L. Altshuler. Supported by EPSRC First Grant EP/E063519/1, the Royal Society, and the Daiwa Anglo-Japanese Foundation.

11:51AM Y3.00002 Quantum interference in Epitaxial Graphene: Evidence for Chiral Electrons. XIAOSONG WU, School of Physics, Georgia Tech — The extraordinary transport properties of graphene originate from its unique band structure. Electrons in the band have chirality, which correlates the directions of the momentum and the pseudospin. This chirality prevents electrons from being back-scattered, hence causing a particular quantum phase coherent phenomenon, called weak-antilocalization. Recent theoretical work suggested that multilayer epitaxial graphene (EG) grown on SiC possesses essentially same band structure as single layer graphene because of the rotational stacking order between layers. We have investigated the magnetoresistance of EG. We found that weak anti-localization manifests itself as a broad cusp-like depression in the longitudinal resistance for magnetic fields 10 mT < B < 5 T. An extremely sharp weak-localization resistance peak at B = 0 is also observed. These features quantitatively agree with graphene weak-(anti)localization theory implying the chiral electronic character of the samples. Scattering contributions from the trapped char ges in the substrate and from trigonal warping due to the graphite layer on top are tentatively identified. The phase coherence length was found about 1 μm at 4.2 K and the main phase-breaking mechanism was e−e scattering.

Supported by NSF-NIRT Grant No. 0404084, NSF-MRI Grant No. 0521041, a grant from Intel, and a USA-France travel grant from CNRS.

12:27PM Y3.00003 Quantum Interference in Single and Bilayer Graphene. ALEXANDER SAVCHENKO, School of Physics, University of Exeter, Exeter EX4 4QL, U.K. — It is known that interference of charge carriers scattered by impurities results in a quantum correction to the conductivity of the two-dimensional (2D) system. This phenomenon of weak localization (WL) is usually seen as a distinct conductance fluctuation, as magnetic field changes the phase of interfering waves. Here we show that quantum interference in graphene – a single layer of carbon atoms [1] – is very different from that in conventional 2D systems. Due to the chiral nature of carriers, it becomes sensitive to different elastic scattering mechanisms. By changing the geometry and quality of samples we show that quantum interference in graphene can take a variety of forms, and that WL is a sensitive tool to detect defects in graphene crystals [2]. We perform a comparative study of WL in single-layers and bilayers. Although the two systems are different in their spectrum (massless and massive fermions, respectively), the carriers in both are chiral. As a result WL in a bilayer is also affected by elastic scattering [3]. Analysis of the magnetoresistance using theories [4] allows us to determine the phase-breaking time as well as times of inter- and intra-valley scattering, which together control WL. They are found at different carrier densities, including the electro-neutral point where the nominal carrier density is zero. We show that in all cases WL is not suppressed, and that the reason for this is strong inter-valley scattering. The study of WL is complemented by AFM imaging of the surface which provides information about the nature of the defects responsible for the different manifestations of WL in graphene systems. In addition to the studies of WL, we perform analysis of universal conductance fluctuations (UCF) in both systems. They have the same physical origin as WL – quantum interference – and are controlled by the same characteristic times. We compare the times found from analysis of WL and UCF.


1:03PM Y3.00004 Experimental studies of conductance fluctuation and tunneling spectroscopy of weakly disordered graphene devices. YING LIU, Department of Physics, The Pennsylvania State University, University Park, PA, 16802 — We measured the conductance fluctuation and tunneling spectra of single-, bi- and trilayer graphene prepared by mechanical exfoliation. Reproducible fluctuations in conductance as a function of applied gate voltage or magnetic field were found in the electric transport measurements. As the Fermi energy was tuned to near the charge neutral point, the amplitude of the conductance fluctuation was suppressed quickly from a value consistent with universal conductance fluctuations, even though the devices were still well within the weakly disordered regime. The physical origin of the observed suppression may be related to the presence of edge states, or puddles of electrons or holes in graphene devices. The tunneling spectra of planar tunnel junctions of micron size were found to exhibit interesting features that evolve with the backgate voltage, temperature, and applied magnetic field. The implications of these observations will be discussed. This work is done in collaboration with Neal Staley, Conor Puls, and Haohua Wang.

1:39PM Y3.00005 Excitations from Filled Landau Levels in Graphene. ANDREW IYENAGAR — Recent experimental progress has allowed the fabrication of graphene, a two-dimensional honeycomb lattice of carbon atoms that forms the basic planar structure in graphite. Graphene exhibits a host of interesting properties that can be understood in terms of a non-interacting system whose single-particle excitations are described by the Dirac equation. What, then, is the role of the Coulomb interactions between electrons in graphene? In this talk, I will present a study of the collective excitations of graphene in the quantum Hall regime. These excitations open a window into the nature of Coulomb interaction effects and may be observable by optical spectroscopy. Such excitations are well-understood in the case of the standard two-dimensional electron gas (2DEG), in which the low-lying collective mode spectrum may be interpreted in terms of a single particle-hole pair bound into a stable exciton by Coulomb forces. Using a similar analysis for graphene, we find that, in spite of the linear electronic dispersion near the Dirac points, the exciton spectrum is qualitatively quite similar to that of the 2DEG. On the other hand, the additional pseudospin degree of freedom strongly changes many-body corrections relative to the 2DEG case. We also find that the presence or absence of certain branches of the exciton spectrum is sensitive to the number of filled spin and pseudospin sublevels. Finally, I will discuss these results in relation to infrared spectroscopy measurements and comment on the screening of the Coulomb interaction in graphene.

Friday, March 14, 2008 11:15AM - 2:15PM –
Session Y4 DCMP: New Symmetries and Excitations in Multiferroics
Morial Convention Center 206
11:15AM Y4.00001 Observation of ferrotoroidic order in LiCoPO₄₁, MANFRED FIEBIG, HISKP, University of Bonn, Nussallee 14-16, 53115 Bonn, Germany — Domains are an essential property of any ferroic material. Three forms of ferroic order (ferromagnetism, ferroelectricity, ferroelasticity) are widely known. It is currently debated whether to include an ordered arrangement of magnetic vortices as fourth form of ferroic order termed ferrotoroidicity [1]. Although there are reasons to do this from the point of view of thermodynamics a crucial hallmark of the ferroic state, i.e., a ferrotoroidic domain structure, has not been observed before. Here ferrotoroidic domains are spatially resolved by optical second harmonic generation in LiCoPO₄ where they coexist with independent antiferromagnetic domains [2]. The origin of ferrotoroidicity in LiCoPO₄ is discussed and the general relation between ferrotoroidicity and antiferromagnetism or spin-spiral magnetism will be highlighted. Their space- and time asymmetric nature relates ferrotoroidics to multiferroics with magnetoelectric phase control and other systems in which space and time asymmetry leads to exciting possibilities for future application.

3Support by the SFC608 of DFG is acknowledged.

11:51AM Y4.00002 Symmetry in Multiferroics, SANG-WOOK CHEONG, Rutgers University — Symmetries govern Nature ubiquitously from the beauty of human faces to the local gauge invariance of quantum field theory. Magnetic order in frustrated magnets can occur without space inversion symmetry. When it relaxes to the magnetically-ordered configuration through exchange-striction, lattice can also loose inversion symmetry, leading to the presence of ferroelectric polarization. In these magnetically-driven ferroelectrics, dielectric properties turn out to be highly susceptible to applied magnetic fields. Both symmetric and antisymmetric exchange coupling can be involved in the exchange-striction. One form of symmetry often broken in Nature is the symmetry between left- and right-handedness. For example, the manner in which light propagates naturally selects one handedness, and is customarily described by a right-handed rule, depicting the relationship among the oscillating electric field, magnetic field and propagation vector of light. Chiral molecules also have a definite handedness, and given the preponderance of chiral molecules, it is not surprising that most complex proteins as well as their constituent amino acids are chiral. What is remarkable however, is that most of naturally occurring amino acids share the same chirality; only left-handedness. Such handedness, or chirality, appears to be a characteristic signature of life. In the multiferroic spinel Co₂FeO₄, conical magnetic order accompanies ferroelectric polarization as well as ferromagnetic moment. The relevant handedness and chirality in the multiferroic state will be also discussed.

12:27PM Y4.00003 Towards a microscopic theory of toroidal moments in periodic crystals¹. NICOLA SPALDIN, Materials Department, UC Santa Barbara — The recent resurgence of interest in magnetoelectric multiferroics has prompted discussion of the relevance of the concept of magnetic toroidal moments in such systems. In particular, the toroidal moment has the same symmetry as the antisymmetric part of the linear magnetoelectric tensor, suggesting a role in mediating coupling between magnetic and electric polarization in multiferroics. In addition, materials in which the toroidal moments are aligned cooperatively – so-called ferrotoroidics – have been proposed to complete the group of primary ferroics. Here we review the basic microscopic and macroscopic definitions of toroidal moments and illustrate the difficulties in evaluating the toroidal moment of an infinite periodic system. We show that periodic boundary conditions give rise to a multivaluedness of the toroidal moment per unit cell, in close analogy to the case of the electric polarization in bulk periodic crystals. We then evaluate the toroidal moments of several multiferroic and magnetoelectric materials (BaNiFe₄O₁₂, LiCoPO₄, GaFeO₃ and BiFeO₃) in the “localized dipole limit”, where the toroidal moment is caused by a time- and space-reversal symmetry-breaking arrangement of localized magnetic moment.

1Collaboration with Claude Ederer, Trinity College, Dublin

1:03PM Y4.00004 Role of Spin current in multiferroic behavior, NAOTO NAGAOSA, Dept. Applied Physics, The University of Tokyo — No abstract available.

1:39PM Y4.00005 Electromagnons in multiferroics¹. ANDREI SUSHKOV, Department of Physics, University of Maryland — Multiferroic materials with simultaneous magnetic and ferroelectric order exhibit strong cross coupling between electric and magnetic phenomena. One important new effect is the strong coupling between the low lying magnetic and lattice excitations to produce spin waves that interact strongly with light by acquiring electric dipole activity from the phonons. As a result, these excitations, which are called electromagnons, produce contributions to the static dielectric constant which appear in the ordered phases and that can be manipulated with an applied magnetic field. This appears to be the origin of the giant magneto-capacitance effect observed in these multiferroics. Predicted more than three decades ago, electromagnons were reliably observed only recently. In my talk, I will discuss electromagnons in two classes of multiferroic materials: RmO₃ and RmN₂O₅ (R = Y, Rare Earth) in which the multiferrocicity derives from different mechanisms. Correspondingly the electromagnons in these two materials systems have characteristically different spectra and selection rules. The electromagnon H-T phase diagrams for Eu₀.75Y₀.25MnO₃, TbMnO₃, TbMn₂O₅ will be presented. I will also discuss the outstanding problems in understanding these novel excitations and the prospects for electromagnons in other materials.

In present and future high performance CMOS devices, the dedicated introduction is Raman spectroscopy, enabling strain and composition determination in silicon structures on the µ-scale with high accuracy. It will be shown for various strained silicon and silicon-germanium film structures, that optical near-field information can be obtained on a scale promising for CMOS device characterization. Local strain measurements are achieved utilizing TERS with metal coated AFM tips positioned in the region of interest. Experimental results of µRaman and of TERS scans for the strain distribution in island and line structures of thin films are discussed as well as possibilities and limitations for further improvement of the spatial Raman resolution.

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12:27PM Y5.00003 Temporal and Spatial Distributions of Water in Ion-Containing Perfluorosulfonic Polymers

EVANGELOS MANIAS, Penn State University — The spatial distribution and the molecular dynamics of water in perfluorinated ionomer polymeric membranes (Nafion 11x in the acid form) were quantified at several hydration levels by Atomic Force Microscopy and Dielectric Relaxation Spectroscopy, respectively. A variety of concurrent AFM modes, including interleave and intermittent contact methods, is necessary to map the water-containing domains on the polymer surfaces, whereas at least two different dielectric relaxation setups are needed to record the range of water dynamics that develop in these systems as the hydration level changes. The competition between sulfonic-group/water attraction and water/water hydrogen-bonding, in addition to confinement effects, give rise to at least three “states” of water, manifested through distinct dynamical behaviors: The fastest process observed was identified as the cooperative picosecond relaxation of free/isotropic, bulk-like water, whereas the slowest process —with microsecond relaxation times— corresponds to water molecules strongly bound to the charged sulfonic groups. An intermediate relaxation, in the picosecond range and about three times slower than those of bulk water, is shown to contain substantial dynamical heterogeneities and most probably corresponds to a variety of local environments that are cumulatively defined as “loosely bound” water. AFM studies, probing the same surfaces at various hydration levels, provides insights on the location and geometry of the water domains that contribute to the various dynamical “states”. Both the spatial and temporal distributions of water are sensitive to the sample preparation conditions, especially with respect to the geometry and dynamics of the “loosely bound” water domains.

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11:51AM Y5.00002 Using Folding Pathways to Predict Protein Structure

KARL FREED, University of Chicago — Since the demonstration that the amino acid sequence of a protein encodes its structure, the prediction of structure from sequence remains an outstanding problem that impacts numerous scientific disciplines. By iteratively fixing secondary structure assignments of residues during Monte Carlo simulations of folding, a coarse grained model without homology information or explicit side chains outperforms current homology-based secondary structure prediction methods. The computationally rapid algorithm also generates tertiary structures with backbone conformations of comparable accuracy to existing all-atom methods for many small proteins, particularly for low homology sequences. Given appropriate search strategies and scoring functions, reduced representations can accurately predict secondary structure as well as three-dimensional structures, thereby increasing the size of proteins approachable by ab initio methods and the accuracy of template-based methods, in particular for sequences with low homology. In addition, we will discuss recent advances in understanding non-linear electrostatic contributions to transfer free energies in continuum electrostatic models.

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11:15AM Y5.00005 Ion- and pH-dependent volume transitions in biopolymer gels

FERENCE HORKAY, Laboratory of Integrative and Medical Biophysics, National Institutes of Health — Swelling and collapse of polyelectrolyte gels are the result of a balance of different interactions that control the osmotic pressure and network elasticity. In biopolymer systems ions often play a central role in determining the phase behavior. For example, DNA condensation induced by multivalent cations is crucial for its packaging. It is known that biological processes, such as nerve excitation and muscle contraction, are mediated by divalent cations. In general, relatively little is known about the interaction between multivalent ions and charged biopolymers due to the lack of an appropriate theory and the absence of a sufficiently broad base of experimental data. Recent experimental observations made by anomalous small-angle X-ray scattering indicate that the spatial extent of the counterion cloud is significantly reduced in the case of divalent ions relative to the monovalent ions. An understanding of ion induced swelling/collapse transition in polyelectrolyte gels may shed light on the mechanism of important physiological processes. We compare the effects of pH, ion strength and counterion valence on the structure and osmotic properties of biopolymer gels. Systematic studies made on DNA gels indicate that monovalent salts gradually reduce gel swelling but do not cause discontinuous volume transition. In dilute suspensions of these particles, we studied the swelling response for different AAc fractions as a function of pH. In the concentrated suspensions, pH-induced particle expansion can cause transitions between fluid, glassy and crystalline phases. Data will be presented on the dynamics of the observed phase behavior.

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1:03PM Y5.00004 Microrheological studies of solvent-response dynamics of polyelectrolytes

VICTOR BREDVIELD, Georgia Institute of Technology — We have developed a dialysis cell for microrheology, which provides unique capabilities for studying microstructural dynamics of macromolecular solutions due to sudden changes in solvent composition (e.g., ionic strength, pH, solvent/cosolvent ratio). The device was used to determine the response of sodium sulphonated polystyrene (NaPSS) solutions of different molecular weights to changes in counterion concentration. In general, polyelectrolyte chains collapse upon addition of counter-ions, but recent numerical simulations by Hsiao and Luijten (PRL 97, 2006) predicted reexpansion at high concentrations of multivalent counterions. We tested and confirmed these predictions for trivalent chloride salts (Al, In, Ti), although the effect is subtle and strongly varies between the cations investigated. Another study employed the dialysis cell to characterize pH-induced swelling and deswelling of colloidal microparticle mixtures of a polyelectrolyte (NaPSS) and a pH-responsive coil (NIPAM-co-PAA) copolymer. The acid copolymer caueses pH-responsiveness, swelling the particles at high pH due to deprotonation. In dilute suspensions of these particles, we studied the swelling response for different AAc fractions as a function of pH. In the concentrated suspensions, pH-induced particle expansion can cause transitions between fluid, glassy and crystalline phases. Data will be presented on the dynamics of the observed phase behavior.

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NSF-DMR-0602877 and ONR-00014-05-1-0614

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Friday, March 14, 2008 11:15AM - 2:15PM – Session Y6 FIAP: Industrial Advanced Characterizations, Morial Convention Center RO4

11:15AM Y6.00001 Local strain analysis for CMOS technology by Raman and Nano-Raman spectroscopy

MICHAEL HECKER, AMD Saxony LLC & Co. KG — In present and future high performance CMOS devices, the dedicated introduction of mechanical strain into active silicon regions is an important challenge to progress technology. For both basic understanding of the structure-strain relationship and for developing improved device structures, local measurement of the strain state has become essential. A promising technique that meets these requirements is Raman spectroscopy, enabling strain and composition determination in silicon structures on the µm-scale with high accuracy. Locally enhanced Raman intensities due to tip enhanced Raman spectroscopy (TERS) can be utilized to downscale the spatial resolution of Raman spectroscopy significantly below the optical diffraction limit. It will be shown for various strained silicon and silicon-germanium film structures, that optical near-field information can be obtained on a scale promising for CMOS device characterization. Local strain measurements are achieved utilizing TERS with metal coated AFM tips positioned in the region of interest. Experimental results of µRaman and of TERS scans for the strain distribution in island and line structures of thin films are discussed as well as possibilities and limitations for further improvement of the spatial Raman resolution.

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3 NSF-DMR-0602877 and ONR-00014-05-1-0614
11:51AM Y6.00002 Hydrogen storage by physisorption on Metal Organic Frameworks, ANNE DAILLY, General Motors, R&D center, CES Laboratory — Cryo-adsorption systems based on materials with high surface area properties have the main advantage that they can store and release hydrogen with fast kinetics and high reversibility over multiples cycles. Recently Metal Organic Frameworks (MOFs) have been proposed as promising adsorbents for hydrogen. These crystallographically well organized hybrid solids resulting from the three dimensional connection of inorganic clusters using organic linkers show the largest specific surface areas of all known crystalline solids. The determination of the relationships between physical properties (chemistry, structure, surface area . . .) of the MOFs and their hydrogen storage behavior is a key step in the characterization of these materials, if they are to be designed for hydrogen storage applications. Excess hydrogen sorption measurements for different MOFs will be presented. We show that maximum hydrogen uptake at high pressure and 77K does not always scale with the specific surface area. A linear correlation trend only apply within a class of specific materials and breaks down when the surface area measurement does not represent the surface sites that are available to H2. The influence of pore size and shape will also be discussed by comparing several MOFs with different structure types. The hydrogen adsorption and binding energy at low pressure are strongly dependent on the metal ions and the pore size.

12:27PM Y6.00003 Characterization of the pore geometry of porous media and the saturating fluids using 2-dimensional diffusion - NMR relaxation measurements, MARTIN DOMINIK HRLIMANN, Schlumberger - Doll Research — No abstract available.

1:03PM Y6.00004 Non-linear Optical Spectroscopy of Interfaces, MOHSEN YEGANEH, ExxonMobil Research and Engineering Co., Corporate Strategic Research — The critical role played by interfaces can be extended to areas such as nanometer size sensors, electronic devices, fuel cells, composite materials, corrosion, lubrication, oil recovery, catalysis, biology, and aqueous environments. The development of superior technologies in these areas can be driven by rapid advances in interfacial science. Second-order nonlinear optical spectroscopy, particularly sum-frequency generation (SFG) spectroscopy, is well suited for advanced characterization of interfaces. It possesses long penetration depths and intrinsic interface specificity. This talk discusses the general principle of SFG spectroscopy as applied in a petrochemical industry with brief examples related to polymer surfaces, aqueous/oxide interfaces and adsorption of molecular additives from liquid onto solid surfaces.

1:39PM Y6.00005 Development of Silicide Contacts for CMOS devices: Advantages of using Synchrotron Radiation, CHRISTIAN LAVOIE, IBM T.J. Watson Research Center — Silicide films have been used for close to two decades as the contact to the source, drain and gate of state-of-the-art complementary-metal-oxide-semiconductor (CMOS) devices. The desired properties for this contact layer have limited the choice of applicable silicides to low resistivity TiSi2, CoSi2 and NiSi. The stringent and evolving requirements in material properties imposed by continuous scaling have forced modifications to current materials or implementation of the following best candidate. The recent conversion from CoSi2 for the 90 nm technology to NiSi in 65 nm technology and beyond represent a good example of the complexity associated with the integration of a new material. The requirements necessary to achieve performance in current devices are so stringent that even a material such as NiSi studied for more than 3 decades exhibited unexpected characteristics in very thin films and in small devices. The use of intense x-ray beams allows for the characterization of such materials in reduced dimensions and has brought to light multiple unknown behaviors. For example, the morphological stability of NiSi is much lower than originally expected, a result of the complexity in the phase sequence, of the strong anisotropy in properties related to the non-cubic crystal structure and of the very peculiar texture of these films. This early thermal degradation of the contacts has been controlled through process optimization and recently through the use of Ni alloys. In this presentation the impact of using intense x-ray sources for materials optimization will be discussed. The access to these powerful setups has allowed the rapid characterization and optimization of large parameter spaces necessary to develop the knowledge for implementation of new materials in state-of-the-art devices.

Friday, March 14, 2008 11:15AM - 2:51PM — Session Y7 DBP DCP: Control of Light with Bacteriorhodopsin

11:15AM Y7.00001 Earle K. Plyler Prize Talk: Stark Realities, STEVEN BOXER, Stanford University — Stark spectroscopy is the effect of an electric field on a spectrum. Measurements of the Stark effect give information on the change in dipole moment and polarizability for a spectroscopic transition. The great majority of Stark effect measurements have been and still are made in the gas phase where spectroscopic transitions are very narrow and a Stark splitting can be readily measured. There are many fewer examples of Stark spectroscopy measurements in condensed phases, largely because of the perceived difficulty of applying a large electric field. While this is the case for liquid samples, where molecular alignment and low breakdown voltages complicate the measurement, it is simple to immobilize the molecule of interest, either by embedding it in a thin polymer film or by freezing the solvent. The latter is completely general and any sample that forms a high quality optical glass, including protein samples, can be studied. In this talk I will present an overview of applications of Stark effects to diverse systems. We divide the phenomenon into two broad classes: classical Stark effects, where the applied field acts as a perturbation shifting a transition; and non-classical Stark effects, where the applied field affects the intrinsic absorption lineshape and/or populations of states. Classical Stark effects provide quantitative information on the dipolar nature of excited states for electronic or vibrational transitions. Once calibrated, the spectroscopic transition can be used to probe electric fields in organized complex systems such as proteins and changes in those fields accompanying mutations, catalysis, ligand binding and folding. Vibrational Stark effects are particularly useful in this context, and this has led to diverse strategies for introducing unique and sensitive probes for electrostatic fields in proteins. Non-classical Stark effects embrace the many effects that electric fields can have on reaction dynamics, particularly involving electron transfer, either photoinduced or in mixed valence systems. For such systems, the electric field can alter the absorption or emission lineshape substantially because the potential surface depends upon the field and the spectrum depends on the shape of the potential. Examples of each type will be presented.
other natural photoreceptors such as pharaonis phoborhodopsin, proteorhodopsin, photoactive yellow protein and the blue light plant photoreceptor phototropin.

During this talk, switching pump intensity, switched probe profile and phase, and relative phase-shift. Optimized conditions for all-optical switching that include optimized time, switching pump intensity, switched probe profile and phase, and relative phase-shift. Optimized conditions for all-optical switching that include optimized

To this end we have studied the integration of a suitably engineered protein, bacteriorhodopsin (BR), with semiconductor optoelectronic devices and circuits. Successful integration will potentially lead to ultrasensitive sensors with polarization selectivity and built-in preprocessing capabilities that will be useful for high speed tracking, motion and edge detection, biological detection, and artificial vision systems. In this presentation we will summarize our progresses in this area, which include fundamental studies on the transient dynamics of photo-induced charge shift in BR and the coupling mechanism at protein-semiconductor interface for effective immobilizing and selectively integrating light sensitive proteins with microelectronic devices and circuits, and the device engineering of BR-transistor-integrated optical sensors as well as their applications in phototransceiver circuits.

Work done in collaboration with Pallab Bhattacharya, Jonghyun Shin, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI; Robert R. Birge, Department of Chemistry, University of Connecticut, Storrs, CT 06269; and György Váró, Institute of Biophysics, Biological Research Center of the Hungarian Academy of Science, H-6701 Szeged, Hungary.

2:15PM Y7.00006 All-Optical Switching in Bacteriorhodopsin Based on Excited-State Absorption

SUKHDEV ROY, Dayalbagh Educational Institute — Switching light with light is of tremendous importance for both fundamental and applied science. The advent of nano-bio-photonics has led to the design, synthesis and characterization of novel biomolecules that exhibit an efficient nonlinear optical response, which can be utilized for designing all-optical biomolecular switches. bacteriorhodopsin (BR) protein found in the purple membrane of Halobacterium halobium has been the focus of intense research due to its unique properties that can also be tailored by physical, chemical and genetic engineering techniques to suit desired applications. The talk would focus on our recent results on all-optical switching in BR and its mutants, based on excited-state absorption, using the pump-probe technique. We would discuss the all-optical control of various features of the switching characteristics such as switching contrast, switching time, switching pump intensity, switched probe profile and phase, and relative phase-shift. Optimized conditions for all-optical switching that include optimized values of the small-signal absorption coefficient (for cw case), the pump pulse width and concentration for maximum switching contrast (for pulsed case), would be presented. We would discuss the desired optimal spectral and kinetic properties for device applications. We would also discuss the application of all-optical switching to low power all-optical computing devices, such as, spatial light modulators, logic gates and multiplexers and compare their performance with other natural photo receptors such as pharaothis phorhodopsin, proteorhodopsin, photoactive yellow protein and the blue light plant photoreceptor photocarepin.

Friday, March 14, 2008 11:15AM - 1:39PM

Session Y8 DFD: Hydrodynamics of Surfaces and Films Morial Convention Center R06
11:27AM Y8.00002 Rheology and Micro rheology of Actin-Lipid Composites at the Air-Water Interface1, 2, ROBERT WALDER, University of California, Irvine, ALEX LEVINE, University of California, Los Angeles, CHRISTOPH SCHMIDT, Third Physical Institute: Biophysics Georg-August-Universität, Goettingen, Germany, MICHAEL DENNIN, University of California, Irvine — We report on the mechanical properties of a composite material that is a combination of a Langmuir monolayer chemically linked to an actin filament network. This composite system is a 2 dimensional analogue of a cellular membrane and is also expected to have interesting nonlinear mechanical properties. To measure these mechanical properties, we employ traditional rheology and have developed unique microrheological capabilities based on an optical tweezer setup combined with a Couette surface rheometer. This combination of techniques will allow the study of both bulk and local mechanical responses of the composite material to external forces. Studying such materials allows us to simultaneously study a biomimetic material that should provide useful insights into the mechanical properties of biological cells, while also providing a 2 dimensional soft matter system to study the properties of semi-flexible polymer networks.

1Supported by NSF-DMR-0354113. R Walder acknowledges support from a travel fellowship from Institute for Complex Adaptive Matter

11:39AM Y8.00003 ABSTRACT WITHDRAWN —

11:51AM Y8.00004 Elasticity and capillarity: wet hairs and origami, JOSÉ BICO, LINGGUO DU, BENOIT ROMAN, PMMH-ESPCI, JEROME GUILLET, ENS, Paris — Capillary forces are responsible for a large range of everyday observations: the shape of rain droplets, the imbibition of a sponge, the clumping of wet hair into bundles. Although they are often negligible on macroscopic structures, surface capillary forces may overcome volume forces at small scales and deform compliant micro-structures. Capillary-induced sticking can prevent the actuation of mobile elements in MEMS, or even cause their collapse. Capillary forces also have important consequences in biology such as the buckling of the airway lumen induced by surface tension, which can eventually cause the lethal closure of lung airways. We will review a few experimental situations where capillary forces are able to deform two types of objects: rods, and thin sheets. For instance, the nanotubes of a “carbon nanotube carpet” self-assemble into conical “teepee” structures after the evaporation of a solvent and can produce intriguing cellular patterns. Similarly macroscopic wet hairs tend to assemble into bundles through a cascade of successive pairings. The comparison of the physical ingredients involved in these phenomena, attracting capillary forces acting against bending elasticity, leads to a characteristic length: a slender structure longer than this “elasto-capillary” length is considerably bent by capillary forces. The case of thin sheets is trickier because of geometrical constrains, which generally leads to singularities.

12:03PM Y8.00005 Flow fields in soap films: effects of surface viscosity and film thickness, VIKRAM PRASAD, ERIC R. WEEKS, Emory University — A soap film is a thin fluid layer (10 nm to 1 microns thick) separated from bulk air phases above and below it by two surfactant monolayers. We measure the flow field in these films by two-particle microrheology, which looks at the correlated Brownian motion of pairs of embedded tracer particles separated by a distance R. In thin soap films with the thickness comparable to the particle size, and with mobile surfactant interfacial layers, this flow field is long ranged. On the other hand, the flow field in a 3D fluid is known to decay as 1/R. We vary the thickness of the soap film, the mobility (surface viscosity) of the interface and the size of the polystyrene probe particles to quantify the transition of the hydrodynamics of the film from quasi-2D to 3D-like behavior.

12:15PM Y8.00006 Effective Viscosity of a Dilute Suspension of Membrane-bound Inclusions, MARK L. HENLE, ALEX J. LEVINE, Department of Chemistry and Biochemistry, University of California, Los Angeles — In 1906, Einstein famously calculated the effective viscosity of a dilute solution of spheres suspended in a viscous solvent [Annalen der Physik 19, 289 (1906)]. In this talk, we consider the two-dimensional analogue of this problem: that is, we calculate the effective viscosity of a dilute suspension of disks embedded in a two-dimensional fluid membrane. The rheological properties of particle-decorated membranes and fluid-fluid interfaces are important in a variety of soft matter systems. For example, the cell membrane contains a suspension of membrane-bound inclusions (e.g. transmembrane proteins, lipid rafts), which modifies the transport kinetics of the membrane. Also, the interfacial viscosity of liquid-liquid interfaces in colloid-stabilized emulsions plays a key role in preventing droplet coalescence. We include the dissipation caused by flows both within the membrane and in the surrounding bulk fluids. When the flows within the membrane dominate the dissipation, the particle suspension effectively shifts the membrane viscosity. Conversely, when flows induced in the bulk fluids dominate the dissipation, the suspension in the membrane shifts the bulk viscosity. In both limits, we obtain simple analytic expressions for the appropriate effective viscosity.

12:27PM Y8.00007 Contact line motions of drying solutions, FRANCOIS LEQUEUX, CECILE MONTEUX, ASTRID TAY, PMMH-ESPCI, EMMANUELLE RIO, LPS/ORSAY, LAURENT LIMAT, GUILLAUME BERTLOOT, ADRIEN DAERR, MSC/PARIS, PMMD/ESPCI/PARIS TEAM, LPS/ORSAY/FRANCE TEAM, MSC/PARIS/FRANCE TEAM — If most the studies on wetting deal with pure liquids in the absence of evaporation, in practical situations, the liquid is often a solution with an evaporating solvent. This is encountered both in coating and in surface cleaning. In that case, the contact line of a solution is the location of many divergent phenomena. The hydrodynamics dissipation diverges at the contact line: 1) the drying rate diverges at the contact line 2) the concentration diverges at the contact line. The coupling of these phenomena leads to complex effect for the contact line motion. We have observed that an advancing contact line of a colloidal suspension exhibit a stick-slip motion. Moreover, for similar reasons in the case of an advancing contact line of a polymer solution, the contact angle exhibit a minimum as a function of velocity – at which the polymer accumulates on a length of typically 5 nm in the vicinity of the contact line. All these phenomena can explained quantitatively using simple scaling arguments that we will present.

12:39PM Y8.00008 Obtaining Reproducible Slip Measurements on Smooth Hydrophobic Surfaces, SEAN P. MCBRIDE, B.M. LAW, Kansas State University — Over the past decade, the world market for microfluidic technologies and applications of such devices has soared. The slip length parameter at the liquid-surface interface of these devices describes how easily a fluid flows over the surface. As microfluidic devices decrease in size, slip becomes very important. Despite the undeniable success of these devices in recent years, the literature illustrates that numerous discrepancies exist for the slip magnitude measured using different experimental methods. As the need for smaller microfluidic devices approaches, the need for the most efficient drop transport. This capillary ratchet mechanism may also find applications in micro scale fluid transport, such as valveless pumping of fluid drops.

1Center for Bits and Atoms, MIT.
12:51PM Y8.00009 Fabrication of non-aging superhydrophobic surfaces by packing flower-like hematite particles, ANMIN CAO, LIANGLIANG CAO, DI GAO, University of Pittsburgh — We demonstrate the fabrication of non-aging superhydrophobic surfaces by packing flower-like micrometer-sized hematite particles. Although hematite is intrinsically hydrophilic, the nanometer-sized protrusions on the particles form textures with overhanging structures that prevent water from entering into the textures and induce a macroscopic superhydrophobic phenomenon. These superhydrophobic surfaces do not age even in extremely oxidative environments—they retain the superhydrophobicity after being stored in ambient laboratory air for 4 months, heated to 800 degree C in air for 10 hours, and exposed to ultraviolet ozone for 10 hours.

1:03PM Y8.00010 Liquid slip probed by second harmonic generation1, DAN LIS, Laboratoire Lasers & Spectroscopies, University of Namur, STEVE GRANICK, BAE SUNG CHUL, Departments of Materials Science and Engineering, Chemistry, and Physics, University of Illinois, SCIENTIFIC EXCHANGE COLLABORATION — Second harmonic generation has been used to probe how a solid surface responds to flow past it. The surface is quartz, the measurements are made in total internal reflection configuration, and comparison of responses to light with s and p incident polarisation allows us to determine the orientation of dye molecules physisorbed before the onset of the shear flow. By monitoring the orientation of the dye at different fluid viscosity and different shear rate, we deduce the surprising relation between shear rate and surface stress.

1:15PM Y8.00011 Determination of Inter-Phase Line Tension in Langmuir Films3, ELIZABETH K. MANN, LU ZOU, Kent State University, JACOB R. WINTERSMITH, ANDREW J. BERNOFF, Harvey Mudd College, JAMES C. ALEXANDER, J. ADIN MANN, JR., Case Western Reserve University, PREM BANSET, EDGAR E. KOOIJMAN, Kent State University — The hydrodynamic response of a thin fluid film, whether a Langmuir monolayer at the air/water interface or a cell membrane, is difficult to model, since it involves the coupling of both bulk and surfaces phases. However, such hydrodynamic response is not only intrinsically critical for transport within the layer, it also provides the major available means to evaluate an important parameter for phase-separated layers, the line tension. We have developed a line-integral formulation of the hydrodynamic response of phase-separated layers with short-ranged forces, and tested it by comparisons between numerical simulations based on this model and experiment. These experiments both validate the model and demonstrate that the line tension can be determined with unprecedented accuracy and precision. Two systems have been studied to date: a simple smectic liquid crystal multilayer and coexistence between phases in binary lipid/cholesterol mixed layers. For the latter case, long-range dipole-dipole interactions are introduced into the model.

1:27PM Y8.00012 ABSTRACT WITHDRAWN –

Friday, March 14, 2008 11:15AM - 2:15PM –
Session Y9 DAMOP: BEC/Matter Optics/Atom Interferometry Morial Convention Center RO7

11:15AM Y9.00001 Phase diagram of a Bose gas near a wide Feshbach resonance, LAN YIN, Peking University — The phase diagram of a homogeneous Bose gas with a repulsive interaction near a wide Feshbach resonance is studied at zero temperature. The Bose-Einstein-condensation (BEC) state of atoms is a metastable state. When the scattering length $a$ exceeds a critical value depending on the atom density $n$, the molecular BEC state becomes a unstable coherent mixture of atoms and molecules. (http://arxiv.org/abs/0710.5318)(cond-mat/0710.5318)

11:27AM Y9.00002 Initial States of BEC mixtures Produced by Cooling in the Presence of a Feshbach Resonance, LAURA HALMO, Georgia Southern University, MARK EDWARDS, Georgia Southern University and NIST — We have studied the types of Bose–Einstein condensate (BEC) mixtures produced as a result of different cooling paths. These results are relevant to a recent experiment in which a mixture of $^{85}$Rb and $^{87}$Rb BECs was cooled in three stages: (1) optical pre–cooling, (2) evaporative cooling in a magnetic trap, and (3) evaporatively cooled in an optical trap. We used that, upon transfer to the optical trap, the state of the mixture of thermal gases can be represented by the superposition of a small number of low–lying trap eigenstates each with high occupation. In this case, the field operator can be approximated as a c–number and its evolution will be governed by the nonlinear Schrödinger equation. We investigated the density profiles that resulted from different initial thermal distributions as well as non–thermal initial distributions. We also performed studies of the effect of varying the $^{85}$Rb/$^{87}$Rb scattering length via a Feshbach Resonance. We found condensate states that differ markedly from the standard Thomas–Fermi ground states of the Gross–Pitaevskii equation.

11:39AM Y9.00003 Interference between atomic Bardeen-Cooper-Schrieffer gases, TUN WANG, Austrian Academy of Science, SUSANNE YELIN, Univ. of Connecticut — We study the interference between two atomic Bardeen-Cooper-Schrieffer (BCS) gases using noise correlations. Fringes as seen in the interference between two Bose-Einstein Condensates (BECs) do not to exist due to the requirement that two BCS gases have to initially overlap to interfere. This requirement results from the fact that the spin up and spin down fermions in a Cooper pair have opposite momenta. Nevertheless, BCS gases still interfere with each other, and their interference patterns share many aspects with those of BECs.

11:51AM Y9.00004 Single and double reflection Michelson atom interferometers in a weakly-confining magnetic trap, RUDRA KAFLE, JAMES STICKNEY, WPI, DANA ANDERSON, JILA, University of Colorado and NIST, ALEX ZOZULYA, WPI — We analyze the operation of a BEC based atom interferometer, where the atoms are held in a weakly-confining magnetic trap and manipulated with diffraction gratings produced by counter-propagating laser beams. A simple analytic model is developed to describe the dynamics of the interferometer. It is used to find the region of parameters corresponding to high values of the interference fringe contrast for both single and double reflection geometries. We demonstrate that for a double reflection interferometer the coherence time can be increased by shifting the recombination time. Finally, we compare the theory with recent experimental realizations of these interferometers and estimate when phase diffusion and finite temperature phase fluctuations become important.

1:15PM Y8.00011 Determination of Inter-Phase Line Tension in Langmuir Films1, ELIZABETH K. MANN, LU ZOU, Kent State University, JACOB R. WINTERSMITH, ANDREW J. BERNOFF, Harvey Mudd College, JAMES C. ALEXANDER, J. ADIN MANN, JR., Case Western Reserve University, PREM BANSET, EDGAR E. KOOIJMAN, Kent State University — The hydrodynamic response of a thin fluid film, whether a Langmuir monolayer at the air/water interface or a cell membrane, is difficult to model, since it involves the coupling of both bulk and surfaces phases. However, such hydrodynamic response is not only intrinsically critical for transport within the layer, it also provides the major available means to evaluate an important parameter for phase-separated layers, the line tension. We have developed a line-integral formulation of the hydrodynamic response of phase-separated layers with short-ranged forces, and tested it by comparisons between numerical simulations based on this model and experiment. These experiments both validate the model and demonstrate that the line tension can be determined with unprecedented accuracy and precision. Two systems have been studied to date: a simple smectic liquid crystal multilayer and coexistence between phases in binary lipid/cholesterol mixed layers. For the latter case, long-range dipole-dipole interactions are introduced into the model.

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11:15AM Y9.00001 Phase diagram of a Bose gas near a wide Feshbach resonance, LAN YIN, Peking University — The phase diagram of a homogeneous Bose gas with a repulsive interaction near a wide Feshbach resonance is studied at zero temperature. The Bose-Einstein-condensation (BEC) state of atoms is a metastable state. When the scattering length $a$ exceeds a critical value depending on the atom density $n$, the molecular excitation energy is imaginary and the atomic BEC state is dynamically unstable against molecule formation. The BEC state of diatomic molecules has lower energy, where the atomic excitation is gapped and the molecular excitation is gapless. However when the scattering length is above another critical value, $n a^3 > 0.0164$, the molecular BEC state becomes a unstable coherent mixture of atoms and molecules. (http://arxiv.org/abs/0710.5318)(cond-mat/0710.5318)

11:27AM Y9.00002 Initial States of BEC mixtures Produced by Cooling in the Presence of a Feshbach Resonance, LAURA HALMO, Georgia Southern University, MARK EDWARDS, Georgia Southern University and NIST — We have studied the types of Bose–Einstein condensate (BEC) mixtures produced as a result of different cooling paths. These results are relevant to a recent experiment in which a mixture of $^{85}$Rb and $^{87}$Rb BECs was cooled in three stages: (1) optical pre–cooling, (2) evaporative cooling in a magnetic trap, and (3) evaporatively cooled in an optical trap. We used that, upon transfer to the optical trap, the state of the mixture of thermal gases can be represented by the superposition of a small number of low–lying trap eigenstates each with high occupation. In this case, the field operator can be approximated as a c–number and its evolution will be governed by the nonlinear Schrödinger equation. We investigated the density profiles that resulted from different initial thermal distributions as well as non–thermal initial distributions. We also performed studies of the effect of varying the $^{85}$Rb/$^{87}$Rb scattering length via a Feshbach Resonance. We found condensate states that differ markedly from the standard Thomas–Fermi ground states of the Gross–Pitaevskii equation.

11:39AM Y9.00003 Interference between atomic Bardeen-Cooper-Schrieffer gases, TUN WANG, Austrian Academy of Science, SUSANNE YELIN, Univ. of Connecticut — We study the interference between two atomic Bardeen-Cooper-Schrieffer (BCS) gases using noise correlations. Fringes as seen in the interference between two Bose-Einstein Condensates (BECs) do not to exist due to the requirement that two BCS gases have to initially overlap to interfere. This requirement results from the fact that the spin up and spin down fermions in a Cooper pair have opposite momenta. Nevertheless, BCS gases still interfere with each other, and their interference patterns share many aspects with those of BECs.

11:51AM Y9.00004 Single and double reflection Michelson atom interferometers in a weakly-confining magnetic trap, RUDRA KAFLE, JAMES STICKNEY, WPI, DANA ANDERSON, JILA, University of Colorado and NIST, ALEX ZOZULYA, WPI — We analyze the operation of a BEC based atom interferometer, where the atoms are held in a weakly-confining magnetic trap and manipulated with diffraction gratings produced by counter-propagating laser beams. A simple analytic model is developed to describe the dynamics of the interferometer. It is used to find the region of parameters corresponding to high values of the interference fringe contrast for both single and double reflection geometries. We demonstrate that for a double reflection interferometer the coherence time can be increased by shifting the recombination time. Finally, we compare the theory with recent experimental realizations of these interferometers and estimate when phase diffusion and finite temperature phase fluctuations become important.
12:03PM Y9.00005 Prospects for a Gradient Magnetometer Atom Interferometer1, FRANK A. NARDUCCI, JON P. DAVIS, Naval Air Systems Command — Atom interferometers form the basis for state-of-the-art sensors, including gravimeters, gravity gradiometers, gyroscopes and atomic clocks. Notably absent from this list are magnetometers, which can have a wide range of applications ranging from military to medical applications. We propose a scheme to realize an atom interferometer gradient magnetometer. We begin by demonstrating a light-pulse magnetic beam-splitter. The analysis is based on a full multi-level 2-laser field Maxwell-Bloch model including state selection rules, polarization selectivity, laser detuning, and Doppler averaging. We then consider an ensemble of atoms subject to a $\pi/2 - \pi - \pi/2$ pulse sequence. The phase of the interference pattern depends on the phase of the action along the classical path and on the phase of the combined laser fields imprinted on the atoms during the pulse sequence. From this analysis, we conclude that, to first order, the phase of the interferometer output is insensitive to the field across the interferometer, but is sensitive to the gradient of the field. Using realizable numbers from existing interferometers, we show that a gradient magnetometer of this type has can have a greater gradient sensitivity than many current magnetic sensors. We discuss the status of our current experiments using ultra-cold atoms.

3Supported by ILIR and IAR grants from the Office of Naval Research

12:15PM Y9.00006 Bose–Josephson Junction with Binary Mixture of Bosonic Atoms, MARK EDWARDS, Georgia Southern University and NIST, JEFFREY HEWARD, Georgia Southern University, INDUBALA SATIJA, George Mason University and NIST, RADHA BALAKRISHNAN, Institute of Mathematical Sciences, PHILLIP NAUDUS, George Mason University — We consider a Bose–Josephson junction consisting of a binary mixture of two weakly coupled Bose–Einstein condensates confined in a symmetric double–well external potential. In a single condensate confined in a double–well potential, when the condensate wavefunction is approximated as a linear combination of the lowest two eigenmodes of the potential, the result is a dynamical system analogous to those that describe the current and phase across a Josephson junction. Josephson oscillations and nonlinear self–trapping are among the effects predicted by this dynamical system. Using the same two–mode approximation, the condensate mixture can be mapped to two coupled, non–rigid pendula. Although the system is found to exhibit periodic dynamics, the tunneling dynamics of the individual components can be periodic, quasiperiodic, as well as chaotic. We also investigate the experimental signatures of these effects and the goodness of the two–mode approximation by solving the coupled Gross–Pitaevskii equations that govern the behavior of the system.

12:27PM Y9.00007 Dynamics of phase separation in cold-atom boson-fermion mixtures1, DMITRY SOLENOV, Department of Physics, Clarkson University, Potsdam, New York 13699-5820, DMITRY MOZYRSKY, Theoretical Division (T-4), Los Alamos National Laboratory, Los Alamos, NM 87545 — We study the kinetics of the first order phase separation transition in boson-fermion cold atom mixtures. At low enough temperatures such a transition is driven by quantum fluctuations responsible for the formation of critical nuclei of a stable phase. Based on a microscopic description of interacting boson-fermion mixtures we derive an effective action for the critical droplet and obtain asymptotic expression for the nucleation rate in the vicinity of the phase transition and near the spinodal instability of the mixed phase. We show that in the former case the transition rate is significantly modified by dissipation due to interaction with fermion excitations. The regimes where quantum nucleation can be experimentally observed in cold atom systems are identified.

1This work is supported by the US DOE

12:39PM Y9.00008 Quantum phases of mixtures of atoms and molecules on optical lattices1, VALY ROUSSEAU, PETER DENTENEER, Institut-Lorentz — We investigate the phase diagram of a two-species Bose-Hubbard model with an additional conversion term, where two particles from the first species can be converted into one particle of the second species, and vice-versa. The model can be related to ultra-cold atoms experiments where Feshbach resonance, used to tune the scattering length, produces long-lived bound states viewed as diatomic molecules. The model is solved exactly by means of Quantum Monte Carlo simulations. We find that the model exhibits an exotic incompressible “Super-Mott” phase where the particles from both species can flow with signs of superfluidity, but with anti-correlations such that there is no global supercurrent.

1This work is part of the research program of the ‘Stichting voor Fundamenteel Onderzoek der materie (FOM)’, which is financially supported by the ‘Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)’.

12:51PM Y9.00009 First order behaviour of Bose Fermi mixtures across a Feshbach resonance, CHARLES MATHY, Department of Physics, Princeton University, FRANCESLA MARCHETTI, Rudolf Peierls Center for Theoretical Physics, University of Oxford, MEERA PARISH, DAVID HUSE, Department of Physics, Princeton University — We analyze the phase diagram of a mixture of bosonic and fermionic atoms, whose interaction is tuned by varying a magnetic field across a Feshbach resonance. To this end, we introduce a two-channel model and study it with a mean field approach. The phase diagram is found to contain both second order and first order phase transitions, which lead to a regime of densities where phase separation is predicted. We explain why our model is consistent with the experimental observation of collapse, which is usually captured by a single-channel model, and discuss in which systems one is most likely to encounter the physics we are describing.

1:03PM Y9.00010 Boson-Fermion mixture and superconducting phases on the honeycomb lattice, DORON BERGMAN, PETER ORTH, KARYN LE HUR, Yale University — We explore theoretically the different phases of a Boson-Fermion mixture in a honeycomb lattice model. With realistic band structure and interactions, we find that much like phonons in a solid, the bosonic atoms induce effective attractive interactions between the fermions. The attractive interactions can then lead to a number of superconducting phases, which we explore. Using a Bogoliubov and mean-field approach, as well as a full RG treatment, we derive the phase diagram. Possible phases of the system include s-wave as well as $p+ip$ superconducting states. We also analyze the nature of the vortices in the different superconducting states, as these are of great interest as a possible realization of emergent non-Abelian statistics. We explain how tuning between different superconducting phases can be achieved in a cold atomic gas realization of this system.

1:15PM Y9.00011 Supersymmetry and Goldstino-like Mode in Bose-Fermi Mixtures, YUE YU, ITP, Beijing, KUN YANG, National High Magnetic Field Laboratory and Florida State University — Supersymmetry is assumed to be a basic symmetry of the world in many high energy theories, but none of the super partners of any known elementary particle has been observed yet. We argue that supersymmetry can also be realized and studied in ultracold atomic systems with a mixture of bosons and fermions, with properly tuned interactions and single particle dispersion. We further show that in such non-relativistic systems supersymmetry is either spontaneously broken, or explicitly broken by a chemical potential difference between the bosons and fermions. In both cases the system supports a sharp fermionic collective mode similar to the Goldstino mode in high-energy physics, due to supersymmetry. We also discuss possible ways to detect this mode experimentally.
1:27PM Y9.00012 Preemptive phase-transitions in multicomponent BECs\footnote{Work supported by Research Council of Norway.}, STEINAR KRAKSET\footnote{Work supported by Norwegian Research Council}
Norw. Univ. of Sci & Tech, ESKIL KULSET DAHL, Norw. Univ. of Sci & Tech, EGOR BABAEEV, University of Massachusetts Amherst, ASLE SUDBO, Norw. Univ. of Sci & Tech — We use analytical arguments and large-scale Monte-Carlo simulations to investigate phase transitions between various complex superfluid phases in a two-component Bose-Einstein condensate with varying non-dissipative drag between the two components. We focus on establishing the phase diagram and in detail the individual and composite superfluid densities that the system features, using a representation in terms of the phases of the superfluid ordering fields. In particular, we describe a novel preemptive scenario, whereby drag induces a first-order transition from the interplay between two phase-transitions that individually would have been in the $3DXY$-universality class. Our results may shed light on similar phenomena occurring in certain multicomponent superconductors and in scenarios of deconfined quantum criticality in certain quantum antiferromagnetic systems.

1:39PM Y9.00013 Chaos Threshold in Bose-Hubbard Model, AMY CASSIDY, University of Southern California,
VANJA DUNJKO, MAXIM OLSHANII, University of Massachusetts Boston — The goal of this work is to determine the criterion for chaos in the one-dimensional mean-field Bose-Hubbard model. We investigate the time evolution of this system with a few low-energy momentum modes excited initially. A threshold for chaos is defined from calculations of the largest Lyapunov exponent, which is compared with the predictions of the Chirikov criterion of overlapping resonances. Additionally, the results are compared with a closely related fully integrable model.

1:51PM Y9.00014 Quantum quench dynamics in analytically solvable one-dimensional models, ANIBAL Iucci, University of Geneva, MIGUEL A. CAZALILLA, Centro de Fisica de Materiales, San Sebastian, Spain, THIERRY Giamarchi, University of Geneva — In connection with experiments in cold atomic systems, we consider the non-equilibrium dynamics of some analytically solvable one-dimensional systems which undergo a quantum quench. In this quench one or several of the parameters of the Hamiltonian of an interacting quantum system are changed over a very short time scale. In particular, we concentrate on the Luttinger model and the sine-Gordon model in the Luther-Emery point. For the latter, we show that the order parameter and the two-point correlation function relax in the long time limit to the values determined by a generalized Gibbs ensemble first discussed by J. T. Jaynes [Phys. Rev. 106, 620 (1957); 108, 171 (1957)], and recently conjectured by M. Rigol et al. [Phys. Rev. Lett. 98, 050405 (2007)] to apply to the non-equilibrium dynamics of integrable systems.

2:03PM Y9.00015 Superconducting-vortex WCP describes the dragging anisotropy quantitatively. This picture is further supported by the observation that vortex motion is more erratic along the $O_3$-chains than across them. The decay and oscillations of the current are analytically derived, and studied numerically along with the momentum distribution after the quench. In the case of small supercurrent boosts $\nu^3$, we find that the current surviving at long times is proportional to $\nu^3$.

Friday, March 14, 2008 11:15AM - 2:15PM
Session Y10 DCMP: Superconducting Nanostructures II Morial Convention Center R08

11:15AM Y10.00001 Studying pinning on the nanoscale by vortex dragging in a YBa$_2$Cu$_{3-\delta}$O$_{9-\delta}$ single crystal, O. M. AUSLAENDER, LAN LUAN, Stanford University, E. ZELDOV, Weizmann Institute of Science, K. A. MOLER, Stanford University, D. A. BONN, RUIXING LIANG, W. N. HARDY, University of British Columbia — We have used a magnetic force microscope to drag individual, well isolated vortices in a detwinned YBa$_2$Cu$_{3-\delta}$O$_{9-\delta}$ single crystal. At this slight degree of overdoping, a vortex can be described as a one-dimensional elastic string. We find an angle dependent dragging distance, implying that it is easier to drag a vortex along the Cu-O chains than across them. We understand this as a manifestation of single vortex weak collective pinning (WCP) by oxygen vacancies across the Cu-O chains, the dominant source of pinning in our sample. Single vortex WCP arises when individual pinning sites are too weak individually, but able to compete with elasticity by cumulative effect. Using the usual single vortex WCP assumption of isotropic point pinning sites at uncorrelated positions we find that the anisotropy of superconductivity in YBa$_2$Cu$_{3-\delta}$O$_{9-\delta}$ only partially accounts for the angle dependence. Relaxing that assumption to account for the known vacuum of the vacancies to cluster along the Cu-O chains, we find that single vortex WCP describes the dragging anisotropy quantitatively. This picture is further supported by the observation that vortex motion is more erratic along the chains than across them.

11:27AM Y10.00002 Fabrication and characterization of YBa$_2$Cu$_{3-\delta}$O$_{7-\delta}$ Aharonov-Bohm rings and ultra-long nanowires, PAICHIA KUO, JESSIE SHUEN, Institute of Physics, Academia Sinica, Taiwan, PATRICK MORALES, J.Y.T. WEI, Dept. of Physics, University of Toronto, Canada — We report a novel technique to fabricate YBa$_2$Cu$_{3-\delta}$O$_{7-\delta}$ (YBCO) nanowires with characteristic length scale smaller than the YBCO penetration depth. The nanowires presented here are Aharonov-Bohm rings $\sim 15 \mu m$ in diameter, and 200 nm nanowires $\sim 300 \mu m$ in length. These devices have TC behaviors similar to that of unpatterned YBCO thin films. Fabrication of nanostructured complex oxide is a challenge even with advanced thin film growth techniques since either chemical or physical etching tends to compromise the film properties. The effective method is to epitaxially deposit thin film onto nano-patterned oxide substrate without any post-deposition treatment. Our novel technique takes advantage of the 3Dmicromachining capability of focused-ion-beam to nano-pattern the oxide substrate without the inherent surface damage and edge rounding problems caused by the energetic ion beam. This method is a reliable way to fabricate nanostructures of complex oxides and hence enables the studies of their properties.

11:39AM Y10.00003 Electrical Transport Properties of Nanostructured YBa$_2$Cu$_{3-\delta}$O$_{7-\delta}$ Rings and Wires\footnote{Work supported by: NSERC, CFI/OIT, Canadian Institute for Advanced Research and Core Facilities for Nanoscience and Nanotechnology (NanoCore) at Academia Sinica Taiwan.}, P. MORALES, J.Y.T. WEI, Dept. of Physics, University of Toronto, P.C. KUO, J. SHUEN, M.K. WU, Institute of Physics, Academia Sinica Taiwan — The resistance and current-voltage characteristics of nanostructured high-$T_c$ superconducting YBa$_2$Cu$_{3-\delta}$O$_{7-\delta}$ rings and wires were studied as a function of temperature and applied magnetic field. The rings and wires were fabricated by pulsed laser deposition of YBa$_2$Cu$_{3-\delta}$O$_{7-\delta}$ on patterned SrTiO$_3$ substrates. The substrates were patterned using two different techniques. The first technique is based on selective epitaxial growth, and the second, using a method based on focused ion beam. Nanostructured superconducting rings were fabricated with a diameter of $1.5\mu m$ with the width of the arms of the rings being 150nm. The low field magnetoresistance of the rings exhibit characteristics indicative of quantum interference effects. Nanostructured superconducting wires were fabricated with lengths up to 300$\mu m$ and widths as small as 200nm. The current-voltage characteristics of the wires exhibit discontinuities under current biasing and $s$-shaped non-linearities under voltage biasing characteristic of the formation of phase slip lines, the 2D analog of phase-slip centers.
11:51AM Y10.00004 Flux and bias driven superconducting to normal transition in an SNS proximity dc SQUID1, JIAN WEI, PAUL CADDEN-ZIMANSKY, VENKAT CHANDRASEKHAR, Northwestern University — We measure the magnetoresistance of a dc SNS SQUID in the form of a mesoscopic normal-metal loop in contact with two superconducting electrodes. Below the transition temperature of the superconducting leads, large $h/2e$ periodic magnetoresistance oscillations can be observed when the normal sections of the SNS junctions enter a proximity regime induced by the superconducting electrodes. As the temperature is lowered, the entire device becomes superconducting. In this regime, sharp switching from the zero-resistance state to a finite-resistance state is seen at half-integer flux quanta. With the application of a dc bias current at even lower temperatures, periodic switching from the superconducting state to the fully normal state can be produced with the external field. The observation of periodic flux-driven transitions in this device suggests that beyond the current SQUID theory for SNS junctions that incorporates the kinetic energy of the coherent electrons in the junctions is needed.

1This work was funded by the NSF through grant DMR-0604601.

12:03PM Y10.00005 Charge and mass of Cooper pairs in small superconducting rings, VICTOR VAKARYUK, University of Illinois at Urbana-Champaign — It is well known that response of a neutral fermionic superfluid to rotation or a superconductor to magnetic field and/or rotation involves such characteristics of a Cooper pair as, stretching terms a little, its mass $2m$ and charge $2e$. Here $m$ and $e$ are essentially bare mass and charge of particles constituting the Cooper pair e.g. electrons in case of superconductors. On a phenomenological level this is a consequence of the fact that expressions for currents are written for pairs of particles. We analyze this situation in BCS framework and show that for superfluids mesoscopically constrained in (at least) one spatial dimension the pair’s mass and charge become smaller than their values in bulk case (i.e. $m$ and $2e$). One of the implications of this result is the absence of $h/2e$ harmonic in the response of small superconducting rings or tubes to external magnetic field.

1ignoring tiny relativistic corrections

12:15PM Y10.00006 Emergence of $h/e$-period oscillations in the critical temperature of small superconducting rings enclosing magnetic flux, T2U-CHIEH WEI, Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, 200 University Ave. W., Waterloo, ON N2L 3G1, Canada, PAUL M. GOLDBART, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, USA — The Little-Parks critical-temperature oscillations, with magnetic flux, of a large-radius hollow cylindrical superconductor have a period $h/2e$. This oscillation period reflects the binding of electrons into Cooper pairs. On the other hand, the single-electron Aharonov-Bohm oscillations in the resistance or persistent current in a clean metallic ring have period $h/e$. By using the Gor'kov approach to BCS theory, we investigate oscillations in the critical temperature of a superconducting ring, for radii that are comparable to the superconducting coherence length. In this regime, oscillations in the critical temperature of period $h/e$ emerge, in addition to the usual Little-Parks-period oscillations. We argue that in the clean limit there is a superconductor-normal phase transition at nonzero flux, as the ring radius becomes sufficiently small, and that this transition can be either second- or first-order, depending on the ring radius and the external flux. In the dirty limit, we argue the transition is rendered second-order, which results in continuous quantum phase transitions tuned by flux and radius.

12:27PM Y10.00007 Current fluctuations in rough Josephson tunnel junctions1, FRANK WILHELM, GEORG HEINRICH, University of Waterloo — The barrier material of superconducting tunnel junction has become the focus of interest as there is evidence that it limits the intrinsic quantum coherence of superconducting qubits. It is also potentially responsible for $1/f$ noise in SQUIDs. We study the model of a “sieve” junction of many opaque transport channels plus few pinholes, modeling a rough tunnel barrier. Even if the pinholes have a small effect on the subgap current, they completely dominate the shot noise at low voltages. Remarkably, even a fully open pinhole contributes shot noise because the size of the charge quantum it carries is uncertain. The full-counting statistics of charge transfer leads to a multimodal distribution. It is discussed, to what extent this distribution can be interpreted as the onset of telegraph or $1/f$ noise. This theoretical work is based on an extensive full counting statistics calculation using Keldysh Green’s function.

1Sponsored by NSERC Discovery Grants, EU EuroSQIP, and the German Studienstiftung.

12:39PM Y10.00008 Josephson effect through a resonant level coupled to a single oscillator model1, MIKAEL FOGELSTROM, JONAS SKOLDBERG, TOMAS LOFWANDER, Dept. of Microtechnology and Nanoscience (MC2), Chalmers University of Technology — Motivated by very recent experiments on superconducting transport through single-walled carbon nanotubes, we investigate the supercurrent through a one-level quantum dot connected to a single phonon mode. Calculations are done using non-equilibrium Green’s function methods within a self-consistent Born approximation, i.e. assuming that the tunneling rate is much larger that the effective electron-phonon coupling. We calculate both the modified Andreev-bound state spectrum and the renormalization of the phonon density-of-states in situations when the phonon-mode is either in or out-off thermal equilibrium with the electron system. Based on our calculations we discuss possible Andreev-state spectroscopy.

1This research was supported by the Swedish Research Council (VR).

12:51PM Y10.00009 Quantum Phase Slips in 1D Josephson Junction arrays, JACK LIDMAR, KTH Stockholm — One-dimensional arrays of Josephson junctions can undergo a zero temperature superconductor-insulator quantum phase transition by tuning the Josephson coupling. Quantum phase slips (QPS) play the key role in this transition. In the superconducting regime they are very rare, while in the insulating Coulomb blockade regime, they proliferate and destroy the phase coherence. We derive an expression for the QPS rate that is amenable to quantum Monte Carlo simulations and perform calculations in a realistic model of an array over a wide range of parameters including the transition region. In particular we can determine the scaling properties of the QPS rate at the transition.

1:03PM Y10.00010 Macroscopic Resonant Tunneling through Andreev Interferometers, JEFF WEISS, University of Arizona, MARLIES GOORDEN, University of Geneva, PHILIPPE JACQUOD, University of Arizona — We investigate the conductance through and the spectrum of ballistic Andreev interferometers, chaotic quantum dots attached to two $s$-wave superconductors, as a function of the phase difference $\phi$ between the two order parameters. A combination of analytical techniques – random matrix theory, Nazarov’s circuit theory and the trajectory-based semiclassical theory – allows us to explore the quantum-to-classical crossover in detail. When the superconductors are not phase-biased, $\phi = 0$, we recover known results that the spectrum of the quantum dot exhibits an excitation gap, while the conductance across two normal leads carrying $N_N$ channels and connected to the dot via tunnel contacts of transparency $T_N$ is $\propto T_N^{\frac{1}{2}} N_N$. In contrast, when $\phi = \pi$, the excitation gap closes and the conductance becomes $G \propto N_N N_N$ in the universal regime. In the tunneling regime, $T_N \ll 1$, resonant contributions induce an order-of-magnitude enhancement of the conductance towards $G \propto N_N^2$ in the short-wavelength limit. We relate this to the emergence of a giant peak in the density of states at the Fermi level. Our predictions are corroborated by numerical simulations.
of the two-component wave form. As their relative phase is undetermined. We report on the use of the phase sensitivity of the transient grating experiment to separate the individual components.

Conventional pump-probe methods have revealed at least two components in the change in transmission. Resolving these components is inherently ambiguous.

Evolution of the amplitude changes in the transmission of $YBa_2Cu_3O_{7-x}$ thin films have been measured using the charge-grating technique. In this technique two non-collinear pulses are interfered to create a sinusoidal spatial variation in superfluid density, which leads to a grating in the transmission coefficient. Evolution of the amplitude and phase of this grating in the time-domain can be monitored by the coherent detection of a time-delayed diffracted probe pulse. Previous experiments using conventional pump-probe methods have revealed at least two components in the change in transmission. Resolving these components is inherently ambiguous as their relative phase is undetermined. We report on the use of the phase sensitivity of the transient grating experiment to separate the individual components of the two-component wave form.

**References:**


**Support from US DOE**
11:27AM Y11.00002 Visible-pump, THz-probe measurement of the photocarrier mobility in an undoped cuprate. J. STEVEN DODGE, Simon Fraser University, RUIXING LIANG, University of British Columbia — We present new experimental results on the mobility of photoexcited carriers in Sr$_2$CuCl$_3$O$_4$, an undoped cuprate. We use ultrafast laser pulses to excite photocarriers in the antiferromagnetic insulating lattice. We then probe the low-frequency dynamical conductivity of the resulting nonequilibrium state with time-domain terahertz spectroscopy. We observe the prompt onset of photoconductivity followed by a non-exponential decay on ps timescales. Assuming all photoexcited carriers are free we observe a peak mobility of ~0.1 cm$^2$/Vs, much lower than the Hall mobility in chemically doped systems with similar carrier concentrations. Such a low mobility suggests the formation of polarons or excitons after photoexcitation. We will also discuss the temperature dependence of the nonequilibrium state.


11:39AM Y11.00003 Time-resolved spectroscopy of the charge-transfer gap in Sr$_2$CuO$_2$Cl$_2$. J. STEVEN DODGE, Simon Fraser University, ANDREAS SCHUMACHER, Lawrence Berkeley National Laboratory, LANCE MILLER, Ames Laboratory, DANIEL CHEMLA, Lawrence Berkeley National Laboratory — We present energy- and time-resolved pump-probe spectroscopy near the charge-transfer gap in the undoped cuprate compound Sr$_2$CuO$_2$Cl$_2$. Upon photoexcitation, an increase in absorption is observed for energies below 1.95 eV, whereas a decrease occurs above 1.95 eV. Overall, the spectral weight is not conserved over the probe range of 1.6-2.3 eV. No hole-burning is observable at the pump energy $E_{pump}=2.1$ eV. The transient spectral changes appear as one spectral unit instantaneously after the excitation, and they decay, again as one spectral unit, on a picosecond time scale. The photoinduced response relates simply to the thermal response, indicating a common boson-mediated origin. These results support a theoretical model that places the gap energy near 1.5 eV, well below the peak in the charge-transfer absorption spectrum. In this model, the photoexcited state decays rapidly to the gap energy via phonon emission, and the presence of the additional phonons then has the same effect on the charge-transfer absorption as an increase in the equilibrium lattice temperature.


11:51AM Y11.00004 Unusual Spectral Signatures in Na-doped Oxychloride High Temperature Superconductors. M. BRUNNER, University of California, Santa Cruz, K.-H. KIM, H.-G. LEE, S.-I. LEE, Pohang University of Science and Technology, M.R. PETERSON, B.S. SHASTRY, G.-H. GWEON, University of California, Santa Cruz — Electron spectroscopy studies on Na-doped oxychloride samples (Na-COC, (NaCa)$_2$Cu$_2$O$_2$Cl$_2$) have received much attention recently, due to the facts that Na-COC samples are easy to cleave, the crystal structure is relatively simple among the cuprates, and the spectroscopy reveals enhanced signatures of putative “competing order.” Here, we report the electronic structure of Na-COC investigated by angle resolved photoelectrode spectroscopy (ARPES) as a function of momentum, energy, and doping, with an emphasis on unusual nature of some signatures clearly observed in this family of the cuprates. We discuss those signatures in relation to the recently discovered high energy dispersion anomaly and the suggested charge order.

12:03PM Y11.00005 Competition scenario in Raman and ARPES experiments in electron-doped cuprates. BELEN VALENZUELA, ELENA BASCONES, Instituto de Ciencias Materiales de Madrid (CSIC) — Raman and ARPES experiments in the superconducting state of electron doped cuprates have shown deviations from the predictions of a monotonic d-wave superconducting gap. Two scenarios have been proposed to explain these experiments: a non-monotonic BCS gap on a large Fermi surface and a two band model due to the truncation of the Fermi surface by antiferromagnetic correlations. We calculate angle resolved photoemission spectrum and Raman signal in the superconducting phase using a two-band model where superconductivity and antiferromagnetism competes and compare our results with others theoretical scenarios. We also discuss the effect of the non-monotonicity of the gap on the tunneling experiments.

12:15PM Y11.00006 Appearance of Universal Metallic Dispersion in a Doped Mott Insulator. HSIN LIN, S. SAHRAKORPI, R.S. MARKIEWICZ, Northeastern U., M. LINDROOS, Northeastern U. and TUT Finland, X.J. ZHOU, Stanford U. and LBNL, T. YOSHIDA, U. of Tokyo, W.L. YANG, Stanford U. and LBNL, T. KAKESHI, U. of Tokyo, H. EISAKI, Stanford U. and U. of Tokyo, S. UCHIDA, U. of Tokyo, SEIKI KOMIYA, CRIEPI Japan, YOICHI ANDO, Osaka U., F. ZHOU, Z.X. ZHAO, Chinese Acad. of Sci., T. SASAGAWA, Stanford U. and TIT Japan, A. FUJIMORI, U. of Tokyo, Z. HUSSAIN, LBNL, Z.-X. SHEN, Stanford U. and LBNL, A. BANSIL, Northeastern U. — Under strong electronic correlations the parent compounds of all cuprate high-temperature superconductors assume the so-called Mott-Hubbard insulating state. By what routes these insulators rapidly to the gap energy via phonon emission, and the presence of the additional phonons then has the same effect on the charge-transfer absorption as an increase in the equilibrium lattice temperature. We present new experimental results on the mobility of photoexcited carriers in Sr$_2$CuCl$_3$O$_4$, a undoped cuprate. We use ultrafast laser pulses to excite photocarriers in the antiferromagnetic insulating lattice. We then probe the low-frequency dynamical conductivity of the resulting nonequilibrium state with time-domain terahertz spectroscopy. We observe the prompt onset of photoconductivity followed by a non-exponential decay on ps timescales. Assuming all photoexcited carriers are free we observe a peak mobility of ~0.1 cm$^2$/Vs, much lower than the Hall mobility in chemically doped systems with similar carrier concentrations. Such a low mobility suggests the formation of polarons or excitons after photoexcitation. We will also discuss the temperature dependence of the nonequilibrium state.

12:27PM Y11.00007 Systematic ARPES study of Ln$_2$Bi$_2$Sr$_{2-x}$CuO$_{6+y}$, ZHIIHUI PAN, MADHAB NEUPANE, YIMING XU, ZIQIANG WANG, Boston College, HUIQIAN LUO, LEI FANG, HAIHU WEN, Institute of Physics and National Lab for Condensed Matter Physics China, HONG DING, Boston College — Ln$_2$Bi$_2$Sr$_{2-x}$CuO$_{6+y}$ is a good candidate to investigate the effects of charge doping and potential disorder to the properties of the high-Tc cuprates. The samples with different Ln elements exhibits very different property, and can used as a probe to study the superconductivity with different Ln substitutions. High-quality single crystals of Ln$_2$Bi$_2$Sr$_{2-x}$CuO$_{6+y}$ have been synthesized over a wide substitution range. We will report our high-resolution ARPES results on of Ln$_2$Bi$_2$Sr$_{2-x}$CuO$_{6+y}$.

12:39PM Y11.00008 Strong correlation effects in the electron momentum density distribution of La$_{2-x}$Sr$_x$CuO$_4$. B. BARBIELLINI, Northeastern U. — NU, P.E. MUNARENS, NU and Delft University of Technology, S. KAPRZYK, NU and AGH, Poland, R.S. MARKIEWICZ, NU, M. ITOU, Y. SAKURAJI, JASRI/Pring-8, Japan, K. YAMADA, Tohoku Univ., Japan, A. BANSIL, NU — Compton scattering offers unique capabilities for measuring absolute spectral weights, which are not obtainable by other spectroscopies. Moreover, this technique is genuinely a bulk-sensitive probe. In this connection, we have carried out a series of high resolution Compton scattering measurements on oriented single crystals of La$_{2-x}$Sr$_x$CuO$_4$ at three different dopings x=0, 0.15 and 0.30, together with corresponding computations based on the LDA and on models for treating strong correlation effects. Theoretical predictions are compared and contrasted with the experimentally reconstructed two-dimensional electron momentum densities to identify strong correlation effects in the spectra, and to delineate how these effects evolve as the system undergoes the transition from the Mott insulator to the superconductor. Work supported in part by the USDOE.
12:51PM Y11.00009 New analysis of the electronic excitations in the Mott insulator Nd$_2$CuO$_4$ using momentum-dependent intensity maps. GUILLAUME CHABOT-COUTURE, Stanford University, JASON N. HANCOCK, Stanford University/SSRL, DIEGO M. CASA, Advanced Photon Source, ANL, PATRICK K. MANG, THOMAS GOG, Advanced Photon Source, ANL, MARTIN GREVEN, Stanford University/SSRL — Resonant inelastic X-ray scattering (RIXS) is a rapidly advancing technique that allows the measurement of electronic excitations in correlated-electron systems. In order to extend this technique, we developed a new circle to perform azimuthal rotations of the crystal. This allowed us to perform precise measurements of the electronic excitations as a function of the momentum transfer in the copper-oxygen planes and the incident photon polarization. As a result, we discovered that Cu K edge RIXS is at most weakly polarization dependent when the polarization is kept in the copper-oxygen planes. We used this new circle to determine the intensity variations of different energy-loss excitations across many Brillouin zones. These intensity maps as well as inelastic spectra measured at high-symmetry points in the Brillouin zone allow an improved analysis of the electronic-excitation spectral weight in this material. We discuss our findings in the context of past measurements on other cuprate systems.

1:03PM Y11.00010 Valence Electronic Structure of YBCO Probed by X-ray Standing Waves. JORG ZEGENHAGEN, SEBASTIAN THIESS, TIEN-LIN LEE, ESRF, CARMELA ARUTA, INFN, Rome, CHENG-TIEN LIN, MPI-FKF, Stuttgart, FEDERICA VENTURINI, NICHOLAS BROOKES, BRUCE C.C. COWIE, ESRF — The photoelectron emission spectrum of the valence band of the high-temperature superconductor YBa$_2$Cu$_3$O$_{6.5}$ (YBCO) in the X-ray regime is dominated by contributions from the copper sites (d states) because of the comparably large cross section. With the help of the x-ray standing wave (XSW) technique in combination with photoelectron spectroscopy, it is possible to separate the contributions to the valence band originating from different lattice sites, even if they are populated by the same element. In this work, by applying the XSW method with photoelectron spectroscopy, we discriminated the contributions to the YBCO valence band coming from the nonequivalent in-plane and chain copper sites. Within the resolution of our measurements, the contributions of Cu-I and Cu-II to the valence band were found to be identical.

1:15PM Y11.00011 Doping Dependence of New Electronic Excitations in La$_{2−x}$Sr$_x$CuO$_4$ Observed by K-edge RIXS. D.S. ELLIS, JUNGO HI, Univ. Toronto, J.P. HILL, Brookhaven National Lab, S. WAKIMOTO, Japan Atomic Energy Research Institute, R.J. BIRGENEAU, Univ. California Berkely, T. GOG, D. CASA, Argonne National Lab, Y.-J. KIM, Univ. Tokyo — Resonant inelastic xray scattering (RIXS) spectra of the cuprate La$_{2−x}$Sr$_x$CuO$_4$ are measured for single crystal samples with progressively larger value of x, ranging from undoped to the overdoped regime. As x is increased in the underdoped region, the lowest energy excitation above the charge transfer gap is sharply suppressed, but many of the general spectral features and overall spectral weight distribution above the gap do not appreciably change, and the broad intensity around the same energy of the exciton remains constant. As the sample becomes overdoped, a much more pronounced change of the spectral weight above the charge transfer gap occurs. An in-gap state at ~1.8 eV in the undoped case, which shows no dispersion with momentum, broadens and shifts down in energy as the doping is increased. The amount of the observed shift is to within an order of magnitude of the change calculated from simple crystal field model.

1:27PM Y11.00012 Charge superstructures in Zn-doped La$_{2-x}$Sr$_x$CuO$_4$. J. C. LEE, University of Illinois, A. RUSYDI, University of Hamburg, S. SMADICI, S. WANG, P. ABBAMONTE, University of Illinois, M. ENOKI, M. FUJITA, Tohoku University, M. RUEBHAUSEN, University of Hamburg, K. YAMADA, Tohoku University. We have observed valence band charge order in both twinned and untwinned samples of La$_{1.95}$Sr$_{0.05}$Cu$_{1.95}$Zn$_{0.05}$O$_4$ with resonant soft x-ray scattering. In the untwinned sample the order was observed to be mainly electronic and centered at the (0,0.084,2) position in reciprocal space, indicating diagonal charge order with period 12a$_o$, where a$_o$ is the orthorhombic lattice parameter. This order has approximately half the wavelength of the magnetic order previously observed with neutron scattering in this system, suggesting a stripe interpretation. Preliminary measurements on a twinned sample revealed four satellites at (0,K,2), where K takes on integer multiples of the value 0.011. Relationships between these effects and the crystal structure of La$_{1.95}$Sr$_{0.05}$Cu$_{1.95}$Zn$_{0.05}$O$_4$ will be discussed. *M. Matsuda, et. al., Phys. Rev. B 73, 140503(R) (2006)

1:39PM Y11.00013 The model high-Tc superconductor HgBa$_2$CuO$_{4+δ}$: a quantitative annealing, transport and magnetic susceptibility study. NEVEN BARISIC, YUAN LI, GUILLAUME CHABOT-COUTURE, YU GUICHUAN, Stanford University, YONGCHAN CHO, Pusan National University, XUDONG ZHAO, Jinlin University, MARTIN GREVEN, Stanford University, GREVEN TEAM — The investigation of the physical properties of high-Tc superconductors (HTSCs) is complicated by several materials-related obstacles. In order to obtain reliable experimental results, homogeneous single crystals are needed, which are difficult to obtain due to chemical and/or electronic disorder. HgBa$_2$CuO$_{4+δ}$ (Hg1201) is a particularly interesting HTSC, since it possesses the highest superconducting transition temperature (Tc=97 K) among single Cu-O layers. Recently, we reported a new recipe for the growth of unprecedentedly large, gram-sized monocrystals of Hg1201 [1]. Here, we demonstrate that it is possible to select samples of the highest quality, with very few vortex pinning centers, and to dope them uniformly over a wide range of hole concentration. Furthermore, we show that those crystals can be cleaved and contacted with high-quality electrical contacts. These results make Hg1201 a particularly interesting model system for extensive experimental investigation. [1] X. Zhao et al., Adv. Mater. 18, 3243 (2006)

1:51PM Y11.00014 ABSTRACT WITHDRAWN —
The relativistic infinite plane, PRESTON JONES, University of Louisiana Monroe — In general relativity there have been several proposals as to what constitutes a uniform field. We give the gravitational field due to an infinite plane with finite mass per unit area, and show that this is the closest general relativistic analog to the Newtonian uniform field. Although we work in 4D we show that the 5D generalization of this solution is the starting point for many current research papers in particle physics and cosmology dealing with infinite extra dimension theories known as brane world models. This physical picture of the brane world models as higher dimensional versions of the general relativistic plane allows one to understand many of the features of these models in simple terms.

Einstein’s 1918 Position on the Role of Ether in Relativity Theory, TOM MORTON, Northrop Grumman Corp — In his 1918 “Dialog about Objections to the Theory of Relativity”, Einstein emphasized the potential applicability of the Ether concept in General Relativity. He noted that “Lorentz brought a rigid substance embodying coordinate systems into play, but SRT denied the existence of all ether concepts. However, GRT is different, and empty space has physical qualities characterized as the components of gravitational potential. This situation can very well be interpreted by speaking of an ether whose state varies from point to point. However, one has to be careful not to attribute to this ether any matter-like properties such as a distinct velocity at each point.” This presentation seeks to identify the qualities required of an ether. Concepts might include ether as a cause of gravity, and as the source medium for the production of electric charge. The ether might conceivably take the form of a diffuse mixture of positive and negative electric charge.

Absolute Planck Values: Moving Beyond the Arbitrary Assignment of Unity, JOHN LAUBENSTEIN, IWPD Research Center — Planck Values provide a valuable tool in efforts to understand basic universal relationships; however, they fall short of having any truly intrinsic value. Planck Values come with the assumption that unity can be assigned to up to five of the fundamental universal constants. While constraining these values to unity may be convenient, it by no means ensures that intelligent life anywhere in the universe would make the same assumptions. Further, the peculiar value of the inverse fine structure constant of 137 suggests that it is naíve to assume that any of the physical constants are equal to unity or any other simplistic number. Through an analysis of gravitation and electrostatic force, the IWPD Research Center has derived a logical argument for a revised set of Planck Values that represent absolute values with true universal significance. Of greatest importance, is a recounted Planck Mass that serves as a truly fundamental unit of mass at the quantum scale. This finding contrasts with the significantly large value associated with the current Planck Mass and provides new information that may be critical in the search to unify General Relativity with Quantum Mechanics.

A Zero free Parameter and Zero Counter Term Requirement Found By Replacing the Gauge Derivative General Covariance with Metric Nontrivial General Covariance in The Dirac Equation, DAVID MAKER, none — We replace the general covariance in the gauge derivatives in the Standard Model (SM) with a metric general covariance. The result is a new Dirac equation pde ($i \gamma^{\mu} \partial_{\mu} \psi + \lambda \omega \psi = 0$) for the electron, where here $i$ is just the spatial component. To illustrate the power of this technique we note here that equivalence principle considerations allow only one type of charge $e$. Therefore, $\lambda = 0$ at $r = 0$ with stability the result. Note also that near $r = 2/\lambda$ for this new Dirac equation gives a azimuthal trifolium, 3 charge shapes; so this ONE charge $e$ (so don’t need color to guarantee this) spends 1/3 of its time in each lobe (fractionally charged lobes), the lobe structure is locked into the center of mass (asymptotic freedom), there are six 2P states (corresponding to the 6 flavors) which are the main properties of quarks! without invoking free parameters. The $S$ matrix of this new pde gives the W and Z as resonances and does not require renormalization counterterms or free parameters thereby restoring sanity to theoretical physics. It is vital that the physics community adopt this method if it is to break out of the 30 years of stagnation created by the confusion caused by these free parameters and counterterms.

The Atomic Model, EVAN RAGLAND, Retired Engineer, Eholo Circle, Diamond Head, MS 39255 — An atomic model atomic model positons concentric electron and nucleus fields spinning together about an empty center. It is alternative to the generally accepted planetary system in which electron point particles orbit about a center clump of nucleon point particles. Introduced in 1922 as an alternative to the standard model of the nucleus it applies scientific space-time knowledge unknown when the standard model was conceived. Originally advanced in the spirit of alternative equivalent it evolved to model the entire atomic structure plus many features of space-time. Structural definitions assume space-time properties of: unification expansion, special relativity, electrical field, magnetic field, spin field, gravity field, and space-time surface effect. Field effects are associated with Faraday lines of force field. Model properties feature symmetry and complementarily. Mass structures of the electron, proton, and neutron atom plus the atomic and nuclear constituents of all elements are developed. In addition the nuclear strong force is defined, the magnetic anomaly explained, etc. Model logic constructs the electron as the complement of the hydrogen (proton) atom.

Proof of the Wave Nature of Plants, ORVIN WAGNER, Wagner Research Laboratory — I assume plants operate with a set of frequencies. These frequencies and the means of these frequencies are equal in all directions. We can then write (w=avh/2 or the the distance between adjacent branches, leaves, etc. The ratios, $v_{v}/v_{h}$, are ratios of small integers for sufficient samplings. For example, for Ponderosa pine the ratio is 3/1 or for delicious apple 4/3. Note that these ratios represent the shape of the tree or other plant and their interactions with gravity. These ratios are derivable by other means such as use the ratio of $\#$ of horizontal needles per unit length from a horizontal sample to the $\#$ of needles per unit length from a vertical sample from p-pine. Or measure the vertical and horizontal velocities. My literature provides many other proofs of the wave nature of plants. I suggest that the waves in relative wave outside of plants (outside 4.9 m/s) are a dark matter related since they travel at such low velocities. See my present web site at home.budget.net/~oeodph.

Post modern physics (a revolution in modern physics), SHAHRAM MALEKZADEH, Assistant Professor — When you make a deep study in Classic and modern physics you will find great and numerous weak points. On the other hand when you want to dismiss a wrong theory you should accept the other maybe incorrect theory so I think that we should write the physics from very beginning. Here I mentioned new theories on each field that can be a start for other scientists. Theories like “cyclone theory” which is about light travel or “matrix theory” which denotes that the materials are not made only atoms but an external capsule named matrix.
Disk systems, and hard sphere system for Hard Sphere Equation of State and First Order Phase Transition. Also to be discussed briefly, is the outlook for the development of the quantum version of RMCS for quantum systems. Suggesting that RMCS may provide a highly efficient computational scheme in contrast to traditional Monte Carlo methods which normally require "large" behavior of the solid phase equation of state. Early results show that RMCS provides accurate results in the fluid phase employing "small" n values, thus discussing the power of RMCS as a materials investigative tool will be tested within the region of first order phase transition as well as for correct asymptotic configurations. RMCS results for the equation of state of the hard sphere system from low densities to densities in the neighborhood of closest packing will be range, with arbitrary inter-particle interactions. RMCS employs a new ensemble, the "nearest neighbor ensemble" involving the PDF for "n" nearest neighbor configurations. The formalism provides a unified description which has metadynamics and canonical sampling as limiting cases. Convergence and errors can be rigorously and easily controlled. The parameters of the simulation can be tuned so as to focus the computational effort only on the physically relevant regions of the order parameter space. The algorithm is tested on the reconstruction of alanine dipeptide free energy landscape. [1] A. Barducci, G. Bussi and M. Parrinello, Phys. Rev. Lett., accepted (2007).

Well-tempered metadynamics: a smoothly-converging and tunable free-energy method, ALESSANDRO BARDUCCHI, GIOVANNI BUSSI, MICHELE PARRINELLO, ETH Zurich — We present [1] a new molecular dynamics algorithm for sampling the canonical distribution. In this approach the velocities of all the particles are rescaled by a properly chosen random factor. The algorithm is formally justified and it is shown that, in spite of its stochastic nature, a quantity can still be defined that remains constant during the evolution. In numerical applications this quantity can be used to measure the accuracy of the sampling. We illustrate the properties of this new method on Lennard-Jones and TIP4P water models in the solid and liquid phases. Its performance is excellent and largely independent on the thermostat parameter also with regard to the dynamic properties. [1] G. Bussi, D. Donadio and M. Parrinello, J. Chem. Phys. 126, 014101 (2007).

Hard-sphere variational CPMD approach, GERALD FAUSSURIER, CHRISTOPHE BLANCARD, CEA, PIER LUIGI SILVESTRELLI, Padova University, CEA COLLABORATION, PADOVA UNIVERSITY COLLABORATION — We present a variational method to determine the free total energy of the electron and ion system using the Gibbs-Bogolyubov inequality and a hard-sphere reference system applied to the quantum molecular dynamics code CPMD. Numerical results and comparisons with quantum molecular dynamics simulations and experiments are presented and discussed for dense and expanded aluminum.

Classical Simulation versus Perturbation Theory of Anharmonicity in 2D Lennard-Jones Triangular Lattice, XIAO SHEN, TAO SUN, JULIE STERN, PHILIP B. ALLEN, SUNY at Stony Brook — Classical molecular dynamics simulation and perturbation theory are two methods that can treat the anharmonicity in solids. Classical molecular dynamics simulation can treat anharmonic effects to high order. Perturbation theory beyond lowest order is difficult, and has convergence issues. However, perturbation theory easily treats the thermodynamic limit, while simulation is necessarily done on a finite system. This raises interesting questions such as whether molecular dynamic simulation will give the correct decay rate when the phonon mean free path is larger than the simulation cell. We try to answer such questions, and explore the limits of both methods, by comparing their results. The system we studied is a two dimensional triangular lattice model with a Lennard-Jones potential.

Dissipation in an electric field-driven synthetic rotary caltrop-based molecular motor, CORINA BARBU, VINCENT CRESPI, The Pennsylvania State University — A molecular caltrop has a three-legged base for attachment to a substrate and a vertical molecular shaft functionalyzed with a dipole-carrying molecular rotor at the upper end. The desired rotational motion of the rotor can generate dissipation when the motor is driven at frequencies which are close to the natural frequencies of soft vibrational modes in the structure or librational of the rotator about field direction. Classical molecular dynamics simulations elucidate the role of these resonances and investigate motor performance under external drive.

Convergence Rates of a Dynamic Monte Carlo Reaction-Free Method for Interacting particles, MARTA GUERRA, MARK NOVOTNY, Physics and HPC2 Center for Computational Sciences, Mississippi State University, HIROSHI WATANABE, NOBUYASU ITO, Department of Applied Physics, University of Tokyo — We calculated the efficiency of a Reaction-Free Monte Carlo method in the limit of low temperatures and/or high densities for d-dimensional particles interacting through a repulsive power-law r^{-d} as well as Lennard-Jones Interactions. Theoretically we find the algorithmic efficiency is proportional to \( \rho^{p/2} T^{-d/2} \) where \( \rho \) is the particle density and T the temperature. For different powers (p) in 1, 2 and 3 dimensions as a function of T and \( \rho \) we report results in agreement with our theoretical predictions


Introducing the Reduced Monte Carlo Scheme (RMCS) with Application for High Substitution of the State and First Order Phase Transition, UDUEZI EDGAL, Old Dominion University, DAVID HUBER, University of Wisconsin-Madison — This is the first demonstration of a novel approach, the “Reduced Monte Carlo Scheme” (RMCS), developed for the investigation of the statistical thermodynamic properties of multi-scale material systems (classical and quantum) over the entire temperature and density range with arbitrary inter-particle interactions. RMCS employs a new ensemble, the “nearest neighbor ensemble” involving the PDF for “n” nearest neighbor configurations. RMCS results for the equation of state of the hard sphere system from low densities to densities in the neighborhood of closest packing will be discussed. The power of RMCS as a materials investigative tool will be tested within the region of first order phase transition as well as for correct asymptotic behavior of the solid phase equation of state. Early results show that RMCS provides accurate results in the fluid phase employing “small” n values, thus suggesting that RMCS may provide a highly efficient computational scheme in contrast to traditional Monte Carlo methods which normally require “large” systems for computation. Also to be discussed briefly, is the outlook for the development of the quantum version of RMCS for quantum systems.
12:39PM Y13.00008 ABSTRACT WITHDRAWN –

12:51PM Y13.00009 Angular momentum form of Verlet algorithm for rigid molecules , MIYABI HIYAMA, CREST, Toyota Central R&D Labs., Inc., TOMOYUKI KINJO, SHIAMI HYODO, Toyota Central R&D Labs., Inc. — We seek to make an algorithm based on the Verlet method which could be applied to non-Hamiltonian and explicit time dependent Hamiltonian systems for rigid molecules. For the first step of this aim, we will propose an algorithm based on the Verlet method for rigid molecules and investigate the characteristics of this algorithm for simple system. In our algorithm, the equations of motion for rigid molecules are integrated by Verlet framework in the angular momentum form. This simple algorithm is named 'the angular momentum Verlet algorithm'. We will show the results of MD simulations for 125 carbon tetrachloride molecules using the angular momentum Verlet algorithm. The relative total energy fluctuations are compared with those using the standard leap-frog and the Gear predictor-corrector algorithms. The energy drift using the angular momentum Verlet algorithm is smaller than that using the leap-frog or the Gear predictor-corrector algorithms, especially in the case of MD simulation with the large time interval.

1:03PM Y13.00010 Absorbing boundary conditions for molecular dynamics and multiscale modeling . S. NAMILAE, D.M. NICHOLSON, P.K.V. NUKALA, Computer Science and Mathematics Division, Oak Ridge National Laboratory, C.Y. GAO, Department of Chemical Engineering, University of Tennessee, Y.N. OSESKY, Computer Science and Mathematics Division, Oak Ridge National Laboratory, D.J. KEFFER, Department of Chemical Engineering, University of Tennessee — We present an application of differential equation based local absorbing boundary conditions to molecular dynamics. The absorbing boundary conditions result in the absorption of the majority of waves incident perpendicular to the bounding surface. We demonstrate that boundary conditions developed for the wave equation can be applied to molecular dynamics. Comparisons with damping material boundary conditions are discussed. The concept is extended to the formulation of an atomistic-continuum multiscale scheme with handshaking between the regions based on absorbing boundary conditions. The multiscale model is effective in minimizing spurious reflections at the interface.

1:15PM Y13.00011 Coupling atomistic molecular dynamics and fluctuating hydrodynamics: shear and sound1. RAFAEL DELGADO-BUSCALIONI, Universidad Autonoma de Madrid, GIANNI DE FABRITIIS, Universidad Pompeu Fabra, Barcelona — Bridging spatio-temporal scales is the main objective of multiscale modeling and one of the hot-topics in the simulation community. However, compared to gas and solid phase, hybrid schemes based on molecular-continuum domain decomposition of the liquid phase are relatively less developed. The present hybrid model (see PRL 97, 134501 and PRE 76, 036709) is the first to include several decisive features: the molecular domain is described with atomistic accuracy (chemical specificity), and it is embedded within a continuum fluid description based on the Landau-Lifshitz fluctuating hydrodynamics equations. The hybrid scheme is thermodynamically consistent (e.g. the MD domain is an open subsystem in agreement with the grand canonical ensemble) and fluctuations of mass, momentum and stress are seamlessly connected across the molecular-continuum interface. As the scheme is based on mass and momentum conservation, it enables to solve shear and sound waves traveling across both domains. Due to its relevance we consider water as working solvent. As a test case, we have studied the reflection of sound waves by a lipid monolayer (DMPC) immersed in aqueous solvent.

1:27PM Y13.00012 Concurrent triple-scale simulation of molecular liquids , MATEJ PRAPROTNIK, Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany & National Institute of Chemistry, Hjaurihova 19, Ljubljana, Slovenia, KURT KREMER, Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, RAFAEL DELGADO-BUSCALIONI, Depto. Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, Campus de Cantoblanco, Madrid, Spain — We present a triple-scale simulation of a molecular liquid, in which the atomistic, coarse-grained and continuum descriptions of the liquid are concurrently coupled. The presented approach successfully sorts out the problem of large molecules insertion in the hybrid particle-continuum simulations and thus opens up the possibility to perform efficient grand-canonical molecular dynamics simulations of open molecular liquid systems.

1:39PM Y13.00013 Averaged Equations for Species Interactions in Binary Particulate Systems , DUAN ZHANG, JIN LIU, Los Alamos National Laboratory — Averaged equations for disperse two-phase flows are relatively well-studied compared to averaged equations for binary particulate systems. Disperse two-phase flows can be viewed as a limit of binary particulate system, in which the continuous phase consists of large amount of small particles, such as molecules, and the disperse phase consists of smaller number of large particles. Therefore averaged equations for disperse two-phase flows provide a guide for the derivation of averaged equations for binary particulate systems. A correct system of averaged equations for binary particulate systems has to recover the averaged equations for disperse two-phase flows in this limit. In this talk it is shown that this can only be done by introducing an interspecies stress in a binary particulate system. Although the framework of deriving the averaged equations is applicable to general particulate systems, numerical simulations are performed for a granular system to study the behaviors of the species exchange force, interspecies stresses and interspecies stress.

2:03PM Y13.00015 A numerical method for miscible two-fluid flow at a large density ratio . SIINA HAAPANEN, Stanford University — A computational algorithm for direct numerical simulation of a binary system of miscible fluids at a large density ratio is described. The method is three-dimensional, with two of the three spatial dimensions periodic. A pseudo-spectral discretization is used in the periodic directions, and an eighth order compact finite difference scheme is utilized in the non-periodic direction. The Mach number of the flow is small, and the equations of motion are integrated forward in time using a fractional step method. A constant coefficient elliptic equation (Poisson equation) is solved to determine the pressure. The method is applied to test problems including the Rayleigh-Taylor instability and a miscible two-fluid shear flow. The accuracy of the method, and its stability at a large density ratio of the fluids are discussed.

Friday, March 14, 2008 11:15AM - 2:15PM

Session Y15 GQI: Focus Session: Quantum Metrology and Control: Fundamental Limits and Applications Morial Convention Center 207

11:15AM Y15.00001 Quantum Enhanced Sensing, Measurement, and Control , SETH LLOYD, MIT — This talk investigates how quantum-mechanical effects such as squeezing and entanglement can be used to enhance the precision and sensitivity of imaging, measurement, and control. Entanglement can give a substantial enhancement to sensitivity even in the presence of high levels of noise and loss.
11:51AM Y15.00002 Environmental Constraints in Practical Photonic Quantum Sensing.¹, YAAKOV WEINSTEIN, GERALD GILBERT, MICHAEL HAMRICK, MITRE Quantum Information Science Group — We report on research directed to problems associated with the propagation of photonic signal states in quantum sensing. Attention is devoted to constraints associated to realistic propagation environments for practical applications of quantum sensing.

¹Research supported by DARPA under MITRE Project 0707D070-QA and by the MITRE Technology Program under grant #07MSR205.

12:03PM Y15.00003 Quantum efficiency of binary-outcome solid-state detectors¹, ALEXANDER N. KOROTKOV, University of California, Riverside — We discuss the definitions of the quantum efficiency for binary-outcome detectors of solid-state qubits, focusing on the subclass of quantum non-demolition detectors. Similar to the previously considered case of linear detectors, the definitions of the quantum efficiency are based on the relation between the ensemble decoherence and the information acquired from the measurement (this information determines the lower bound for the ensemble decoherence). Quantum efficiency is analyzed for several models of binary-outcome detectors, including indirect projective measurement, linear detector in a binary-output regime, detector for a phase qubit, and detector based on tunneling into continuum.

¹supported by the DTO/ARO grant

12:15PM Y15.00004 Quantum Metrology with Product States¹, ANIMESH DATTA, SERGIO BOIXO, University of New Mexico, STEVEN FLAMMIA, Perimeter Institute, Waterloo, ANIL SHAJI, CARLTON CAVES, University of New Mexico, EMILIO BAGAN, Universitat Autònoma de Barcelona — We study the performance of initial product states of $n$ of New Mexico, STEVEN FLAMMIA, Perimeter Institute, Waterloo, ANIL SHAJI, CARLTON CAVES, University of New Mexico, EMILIO BAGAN, Universitat Autònoma de Barcelona — We study the performance of initial product states of $n$-body systems in generalized quantum metrology protocols that involve estimating an unknown coupling constant in a nonlinear $k$-body ($k \ll n$) Hamiltonian. We obtain the theoretical lower bound on the uncertainty in the estimate of the parameter. For arbitrary initial states, the lower bound scales as $1/n^2$, and for initial product states, it scales as $1/n^{n-1/2}$. We show that the latter scaling can be achieved using simple, separable measurements. We formulate a simple model, based on the evolution of angular-momentum coherent states, which explains the $O(n^{-3/2})$ scaling for $k = 2$, implementable with short-time measurements. The model shows that the perturbative expansion generated by the quadratic Hamiltonian does not play a role in the enhanced sensitivity scaling. We show that phase decoherence does not affect the $O(n^{-3/2})$ sensitivity scaling for initial product states.

¹Office of Naval Research No. N00014-07-1-0304

12:27PM Y15.00005 Efficient feedback controllers for continuous-time quantum error correction. ANDREW LANDAHL, BRAD CHASE, J.M. GEREMIA, University of New Mexico — We present an efficient approach to continuous-time quantum error correction that extends the low-dimensional quantum filtering methodology developed by van Handel and Mabuchi [quant-ph/0511221 (2005)] to include error recovery operations in the form of real-time quantum feedback. We expect this paradigm to be useful for systems in which error recovery operations cannot be applied instantaneously. While we could not find an exact low-dimensional filter that combined both continuous syndrome measurement and a feedback Hamiltonian appropriate for error recovery, we developed an approximate reduced-dimensional model to do so. Simulations of the five-qubit code subjected to the symmetric depolarizing channel suggests that error correction based on our approximate filter performs essentially identically to correction based on an exact quantum dynamical model.

12:39PM Y15.00006 Passive Cooling of a Micromechanical Oscillator with a Resonant Electric Circuit. K.R. BROWN, J. BRITTON, R.J. EPSTEIN, J. CHIAVERINI, D. LEIBFRIED, D.J. WINELAND, NIST Boulder — Currently there is considerable interest in the cooling of macroscopic mechanical oscillators, as strong cooling may allow one to reach the quantum regime of such oscillators. Recent advances in fabrication and cooling techniques have brought this regime much closer. Here we present theoretical and experimental results for cooling of the fundamental mode of a miniature cantilever by capacitively coupling it to a driven rf resonator circuit. Cooling results from the rf capacitive force, which is phase shifted relative to the cantilever motion due to the finite decay time of the resonant circuit. If this force varies with an appropriate phase shift relative to the motion of the cantilever, it can oppose the velocity of the cantilever, leading to cooling. We demonstrate this technique by cooling a 7 kHz cantilever from room temperature to 45 K, obtaining reasonable agreement with a model for the cooling, damping, and frequency shift. Extending the method to higher frequencies in a cryogenic system could enable ground state cooling and may prove simpler than related optical experiments in a low temperature apparatus.

12:51PM Y15.00007 Sensitive orthogonal optical monitoring of a micromechanical oscillator. AKO CHIJIOKE, JOHN LAWALL, National Institute of Standards and Technology, Gaithersburg, MD — Optical sensing of oscillations of a mechanical microresonator is of crucial interest for a number of purposes including observation of quantum behavior of macroscopic objects and force microscopy. The majority of optical sensing schemes use light aligned with the axis of mechanical oscillation. We present sensitive monitoring of the oscillations of a micromechanical resonator orthogonal to the field in an optical cavity, and its particular advantages.

1:03PM Y15.00008 Sideband Resolved Cooling of a Nanomechanical Resonator Parametrically Coupled to a Microwave Resonator. JARED HERTZBERG, Department of Physics, University of Maryland, TRISTAN ROCHELEAU, TCHEFOR NDUKUM, KEITH SCHWAB, Department of Physics, Cornell University — We have created a nanostructure formed by a radio-frequency nanomechanical (NEMS) resonator capacitively coupled to a 5 GHz superconducting, co-planar waveguide (CPW) resonator. Recently, we have shown that it is possible to passively cool a NEMS resonator to within a few tens of quanta of its ground state, $N = 25$ [1]. By driving this coupled system at a frequency $\omega_{pump} = \omega_{CPW} - \omega_{NEMS}$, we expect to produce an active cooling process in the sideband resolved limit which in principle [2] should be capable of preparing the ground state of motion, with occupation factors $N_{\parallel} 1$. In future work, we expect to be able to demonstrate backaction evading position detection and ultimately squeezed quantum states of the mechanical device by using more advanced pumping schemes, such as double sideband pumping. [1] A. Naik et al, Nature 443, 193 - 196 (2006) [2] F. Marquardt et al, Phys. Rev. Lett. 99, 093902 (2007)

1:15PM Y15.00009 Parametric Amplification of Quantum Signals with a Josephson Ring Modulator. NICOLAS BERGEAL, FLAVIUS SCHAKERT, MICHAEL METCALFE, VLADIMIR MANUCHARYAN, RAJAMANI VIJAYARGHAVAN, MARKUS BRINK, MICHEL DEVORET, Yale University Applied Physics — Quantum Mechanics puts a limit on how small the degradation of information passing through a phase preserving amplifier can be. It is known theoretically that the minimum noise added by the amplifier to the signal amounts at least to half a photon at the signal frequency. Is it possible to construct a practical amplifier working at microwave frequencies that would reach this quantum limit? We have developed a new device aiming at answering this question, which is of practical importance for the readout of solid state qubits, and more generally, for the measurement of very weak signals in various areas of science. The device is based on a ring of four Josephson junctions which connects two microwave resonators corresponding to the signal and idler modes. It can be operated both as an amplifier and a frequency converter. Theoretical aspects and experimental results will be presented.
1:30PM Y18.00011 Impact of Atomic Gap Size on Sensitivity and Backaction of APC Displacement Detectors, N.E. FLOWERS-JACOBS, K.W. LEHNERT, JILA, NIST and the University of Colorado, and the Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA — Recently our group created a mesoscopic displacement detector formed by coupling an atomic point contact (APC) to a nanomechanical beam and demonstrated a displacement imprecision limited by the fundamental shot-noise in the number of electrons that tunnel across the APC [1]. We continue this work by using a cryogenic apparatus that flexes the device substrate to mechanically adjust the size of the APC atomic gap 	extit{situ}. The resulting changes in the APC displacement detector’s intrinsic noise properties are measured by observing the 1 K random thermal motion of the nanomechanical beam at resonance frequencies up to 200 MHz. The goal of this work is to explore the effect of atomic gap size and shape on displacement sensitivity, understand the origin of the observed measurement backaction, and measure the recoil force of tunneling electrons. [1] N. E. Flowers-Jacobs, D. R. Schmidt, and K. W. Lehnert, \textit{Phys. Rev. Lett.} \textbf{98}, 096804 (2007)

1:51PM Y18.00012 Quantum Zeno Effect in Detection of Itinerant Microwave Photons, FERDINAND HELMER, Arnold Sommerfeld Center for Theoretical Physics, Physics Department, Center for NanoScience, Ludwig-Maximilians University Munich, Germany, MATTEO MARIANTONI, Walther Meissner Institut, Bayerische Akademie der Wissenschaften, Garching, Germany, ENRIQUE SOLANO, FLORIAN MARQUARDT, Arnold Sommerfeld Center for Theoretical Physics, Physics Department, Center for NanoScience, Ludwig-Maximilians University Munich, Germany — We analyze detection of itinerant photons using a QND measurement. We show that the backaction due to the continuous measurement poses a fundamental limit for the fidelity of detection in such a scheme. We illustrate this using a setup where signal photons have to enter a cavity in order to be detected dispersively. The measurement signal in this approach is the phase shift imparted to an intense beam passing through a second cavity mode. The restrictions on the fidelity are a consequence of the Quantum Zeno effect, and we discuss both analytical results and quantum trajectory simulations of the measurement process. Finally, we briefly mention a possible experimental realization in the context of superconducting circuit QED.

2:03PM Y18.00013 Rapid Purification protocols for Optical Homodyning, ARAVIND CHIRUVELLI, Louisiana State University, KURT JACOBS TEAM — Recently Jacobs (PRA 67 030301 (2003)) and Wiseman and Ralph (New J. Phys 8, 90(2006)) have discovered rapid purification protocols for a qubit using quantum feedback. We present these protocols in optical setting. These could also be very useful in quantum state preparation for various uses in metrology and control.

Friday, March 14, 2008 11:15AM - 2:03PM

11:15AM Y18.00001 The effect of confinement on the structure of polystyrene melt films, MRINMAY K. MUKHOPADHYAY, SUNIL K. SINHA, University of California, San Diego, CA 92093, LAURENCE B. LURIO, CURT DECARO, Northern Illinois University, DeKalb, IL 60115, ZHANG JIANG, MICHAEL SPRUNG, Advanced Photon Source, Argonne, IL 60439 — The structure factor of thin, Si supported, polystyrene films has been measured using grazing incidence wide angle diffuse x-ray scattering. Measurements were made as function of thickness and molecular weight from bulk-like films down to films of thickness of the polymer radius of gyration. A standing wave technique was employed to isolate the scattering component from the film interior. We observe a diffuse background and a liquid scattering ring whose intensity, for thick films, depends only on the magnitude of the scattering vector. In thinner films the intensity in the scattering ring is strongly concentrated along the surface normal direction. We interpret this peak as due to the chain-chain correlations and the concentration of scattering along the surface normal is indicating preferential stacking of the polymer chains parallel to the surface.

11:27AM Y18.00002 Tuning the Glass Transition Temperature over 100 K using Polymer-Polymer Interfaces, CONNIE B. ROTH, Dept. of Physics, Emory University, RODNEY D. PRIESTLEY, SOYOUNG KIM, Dept. of Chemical and Biological Eng., Northwestern University, JOHN M. TORKELSON, Dept. of Chemical and Biological Eng. and Materials Sci. and Eng., Northwestern University — During the past decade considerable research has focused on the impact of the free surface and substrate interactions on the glass transition temperature (Tg) in nanoconfined geometries. For example, the large (up to 80 K) Tg reductions that have been observed in free-standing films indicate that we still have much to learn about the nature of the glass transition. Here we focus on an entirely different kind of interface, a polymer-polymer interface, which we show can have an even stronger impact on the Tg dynamics than a free surface. We demonstrate that the interactions across a narrow polymer-polymer interface are sufficient to tune the Tg of a single polymer material by over a 100 K simply by changing the type of polymer in the adjoining layer. The cooperative segmental dynamics of the two immiscible polymers are strongly coupled over length scales of several tens of nanometers. These results have significant impact on our understanding of the glass transition in multilayer films and nanostructured polymer blends with large amounts of polymer-polymer interface. These findings also suggest new methods for controlling polymer properties in nanoconfined geometries.

11:39AM Y18.00003 The viscoelastic properties of ultrathin polymer films as measured with a novel nanobubble inflation technique, PAUL O'CONNELL, GREGORY MCKENNA, Texas Tech University — Using a nanobubble inflation technique developed within our laboratory, we have measured the absolute biaxial compliance of polymer films as thin as 11.3 nm. Previous results have shown that the degree of reduction in Tg with film thickness is not universal viz., PVAc shows no reduction even for the thinnest films while the PS shows a significant reduction at a thickness below approximately 80nm. In addition the rubbery plateau region for both materials shows dramatic stiffening as the thickness is reduced (<300 times) and scales as approximately the square of film thickness. We have extended the analysis of the data to directly determine the creep compliance function from the measured data rather than the minimization routine used previously. Creep compliance master curves constructed from data at varying thicknesses show that time-temperature superposition is valid even at the thinnest film thickness. The temperature-time shift factors are consistent with a WLF-type dependence and indicate a reduction in Tg for PS at 11.3nm of 53K while no significant reduction (< 3K) is seen for PVAc.
11:51AM Y18.00004 Fabricating Nanoscale Gratings with Gradient Pattern Height by Annealing Imprinted Polymer Patterns

YIFU DING, HYUNWOOK RO, JIRUN SUN, JING ZHOU, SHENG LIN-GIBSON, CHRISTOPHER SOLES, Polymer Division, National Institute of Standards and Technology — The evolution of nanoimprinted polymer patterns during isothermal annealing is driven by the interplay of the pattern features, material properties of the polymer, and the polymer/substrate interactions. With proper control of these factors, a range of hierarchical nanostructures can be fabricated through thermal annealing of the imprinted polymer patterns. Here we demonstrate an example of creating polystyrene (PS) gratings with gradient pattern height. This is achieved by annealing the imprinted PS gratings under a temperature gradient. In the simplest case, the pattern decay rate is determined by the viscosity and surface tension of the PS. Consequently, the degree of the gradient pattern height can be well controlled through the “fragility” of the PS, i.e., its temperature dependence of the viscosity. Such a gradient grating is extremely useful in the combinatorial studies of the effect of the surface topology on the cell behaviors and controlled wettability.

12:03PM Y18.00005 Substrate and chain size dependence of near surface dynamics of glassy polymers

DONGPING QI, University of Waterloo, ZAHRA FAKHRAAI, JAMES FORREST, University of Waterloo — We report on the application of nanohole relaxation technique to study the surface relaxation of i-PMMA thin films. This allows us to obtain the time dependent relaxation function at a number of different sample temperatures for the first 2-3 nm of the free surface. By studying the film thickness dependence of the near-free surface relaxation for films on different substrates we are able to determine the range over which the substrate directly affects the free surface relaxation. This also allows us to determine a limiting thickness where the free surface relaxation is not affected by the substrate. For such films we determine the Mw dependence of the near free surface relaxation time and find a surprising linear Mw dependence. The Mw dependence is discussed in terms of possible motions as well as polymer configurations near the free surface.

12:15PM Y18.00006 Molecular Simulation of Confined Polymer Films: Structure, Dynamics and the Glass Transition

VIKRAM KUPPA, GREGORY RUTLEDGE, Massachusetts Institute of Technology — Molecular Dynamics simulations are used to probe the structure and dynamics of polymers in extreme confinements. The simulations mimic intercalated nanocomposites in which polymer chains are trapped in nanometer sized slit pores between layered inorganic surfaces: our system consists of thin films of bead-spring chains spatially restricted in one dimension by surfaces comprised of monomer beads arranged in an FCC configuration. The responses of the system are studied as a function of slit spacing, polymer-wall interaction strength and temperature. The glass transition temperatures, as well as the fragility of the confined films are seen to increase with increasing confinement and with increasing attraction of the polymer with the confining wall.

12:27PM Y18.00007 Probing Relaxation in Glassy Freestanding Diblock Copolymer Films

ADAM N. RAEGEN, ANDREW B. CROLL, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University — We employ an axi-symmetric deformation and modulus test (ADAM) to measure the response of a thin freestanding diblock copolymer film to an external load. The method measures the deformation of a spin cast film when an axi-symmetric load is applied by a flat circular punch. The flat punch minimizes uncertainties in the experiment, while the use of spin cast films provides a very smooth contact surface. The use of diblock copolymers allows us to change the internal structure of the film from disordered to ordered (lamellar) and surface topography (flat if there are an integer number of lamellae, and islands, bicontinuous or holes for non-integer) by changing the annealing history and thickness of the sample. We discuss our results in terms of the elastic modulus and creep compliance of the films.

12:39PM Y18.00008 Ellipsometric Investigation of the Surface Dynamics of a Polymer Film near the Glass Transition Temperature

ASHIS MUKHOPADHYAY, CHRISTOPHER GRABOWSKI, Wayne State University — We have investigated the surface dynamics of poly (butyl methacrylate) films by using a phase-modulated ellipsometer, which can measure thickness at angstrom-level resolutions. Experiments were performed for a range of temperatures, both above and below the glass transition temperature (Tg) of this system. Thickness-thickness correlation functions were calculated at each temperature using ellipsometry data collected at 200 Hz frequency. Our results indicate that, above Tg, the relaxation time stays relatively constant (∼1 sec) and the correlation functions obey a simple exponential decay. As Tg is approached, a dramatic increase in the relaxation time is observed and the correlation functions are best fitted with a stretched exponential Kohlraush-Williams-Watts (KWW) relation.

1:03PM Y18.00010 Suppression of the Tg-Confinement Effect in Thin Polymer Films by the Presence of an Anti-Plasticizer

SOYOUNG KIM, MANISH MUNDRA, CONNIE ROTH, JOHN TORKELSON, Northwestern University — The effect of film thickness on the glass transition temperature (Tg) of poly(vinyl acetate) supported on silica was studied via ellipsometry for films that were in the bone-dry state and also with several weight percent water sorbed into the film. The presence of water resulted in a decrease of the Tg of bulk poly(vinyl acetate) films but an increase in the density of the films. This combination of effects indicates that water acts as an anti-plasticizer in poly(vinyl acetate). We demonstrate that the bone-dry poly(vinyl acetate) films exhibit a significant reduction in Tg with decreasing film thickness below about 50 nm. In contrast, the poly(vinyl acetate films) containing several weight percent water exhibited no reduction in Tg relative to bulk Tg with decreasing film thickness down to a thickness of about 10 nm. These results are in accord with recent theoretical analysis (Riggelman et al., PRL 97, 045502 (2006)) indicating that the presence of anti-plasticizers leads to a suppression of confinement effects on the behavior of polymer films and indicate that caution should be employed when studying confinement effects in polymer systems that may sorb significant levels of water from the atmosphere.

1:21PM Y18.00011 Polymer Wall Interactions and Dynamics in Confinements

BOOA RAM CHANDRA, SUDHAMAS MITRA, VIKRAM KUPPA, GREGORY RUTLEDGE, Massachusetts Institute of Technology — Molecular Dynamics simulations are used to probe the structure and dynamics of polymers in extreme confinements. The simulations mimic intercalated nanocomposites in which polymer chains are trapped in nanometer sized slit pores between layered inorganic surfaces: our system consists of thin films of bead-spring chains spatially restricted in one dimension by surfaces comprised of monomer beads arranged in an FCC configuration. The responses of the system are studied as a function of slit spacing, polymer-wall interaction strength and temperature. The glass transition temperatures, as well as the fragility of the confined films are seen to increase with increasing confinement and with increasing attraction of the polymer with the confining wall.

1:45PM Y18.00012 Dynamic response of polymers near glass transition

JING, CHRISTIAN FRETIGNY, CNRS, PPMD TEAM — Dewetting experiments of thin polystyrene films on a liquid substrate are performed in the vicinity of the glass transition. It is shown that this technique reveals the extensional creep compliance function of the polymer. The viscosity in the flow regime is very much reduced when the film thickness becomes comparable to the gyration radius of the polymer. This long time behaviour may be associated with the large length scales involved in the viscous flow which should be modified by confinement. On the contrary, the rubbery plateau remains unaffected by the confinement up to a fraction of the coil size. This can be related to the short length scales involved in the rubber elasticity. In the viscoelastic region, physical aging of the sample is clearly evidenced: Structural recovery complicates the short times dewetting response. Preliminary results are presented of the confinement effects on aging properties of ultra thin films as revealed in this original way.
1:15PM Y18.00011 New Measurements of the Effects of Confinement on the Glass Transition Temperature of Freely Standing Polymer Films  
JOHN TORKELSON, SOYOU NG KIM, CONNIE ROTH, Northwestern University — Pioneering work by the Dutcher group (PRL 77, 2002 (1996)) a dozen years ago led to the first measurement of the T<Tg effect in freely standing polymer films. Their studies were especially intriguing because of the observations of very large Tg reductions relative to bulk Tg and a strong molecular weight dependence of the Tg-confinement effect. Such a molecular weight dependence is absent in the Tg-confinement effect of supported polymer films. Because of experimental difficulties associated with freely standing films, especially when the films are less than 100 nm thick, only a few related experiments have been reported by other research groups. Here we describe new results involving the measurement of Tg via the temperature dependence of fluorescence intensity of dyes labeled at trace levels to the polymer chains. Present measurements on freely standing films of poly(methyl methacrylate) (PMMA) have demonstrated reductions in Tg relative to bulk values of 20 to 25 K in films of 25-40 nm thickness. Tg reductions of at least 5 K are observed when PMMA films are 80 nm thick. Studies are also underway with polyurethane films and with polymers of different molecular weight.

1:27PM Y18.00012 Glass transition in ultra thin polymeric films measured by differential AC-Chip calorimetry  
H. HUTH, A. MINAKOV, C. SCHICK, University of Rostock, Institute of Physics, Uniplate 3, 18051 Rostock, Germany — The film thickness dependence of glass transition in polymer films is still controversially discussed. For different experimental probes different dependencies are observed and a generally accepted link to molecular mobility is not yet established. Calorimetry has proven to provide useful information about glass transition, because it establishes a direct link to energetic characterization. In several cases a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible giving further insights. For thin films in the μm...nm range standard calorimetric methods are mostly not applicable. In the recent years there are new developments in the field of calorimetry which overcome these limitations. We set up a differential AC-chip calorimeter capable to measure the glass transition in nanometer thin films with pJ/K sensitivity. Changes in heat capacity can be measured for sample masses below one nanogram even above room temperature as needed for the study of the glass transition in nanometer thin polymeric films. The glass transition in thin films was determined at well defined experimental time scales. No thickness dependency of the glass transition temperature was observed within the error limits - neither at constant frequency nor for the traces in the activation diagrams.

1:39PM Y18.00013 Relaxation Kinetics of Nanostructures on Polymer Surface: Effect of Orientation, Spacial Confinement, and Chain Mobility  
H.G. PENG, Y.P. KONG, A.F. YEE, Depart. of Chemical Engineering and Materials Science, Univ. of California, Irvine — Nanostructures provide an opportunity for studying relaxation and chain dynamics of polymers when the radius of gyration is not small compared with the dimension of the structure. PS (PDI=1.03-1.05, Mw=6.4 to 1571 kg/mol) gratings of varying line-widths (600 nm, 270 nm, and 30 nm) were fabricated by nanoimprint lithography. When annealed at T ~ bulk Tg, the grating height monitored with an AFM relaxes as surface tension and other driving forces overcome the polymer viscosity. The temperature for rapid relaxation decreases as the feature size diminishes for all molecular weights (MWs), but a simple explanation based on surface enhanced mobility fails to explain the results. The residual molecular orientation effect is identified as the main relaxation driving force for gratings of MWs much larger than the entanglement MW. Comparison between the various nanostructure sizes allows to observe the spatial confinement effect and to determine whether a thin mobile surface layer exists.

Friday, March 14, 2008 11:15AM - 2:03PM  
Session Y22 DPOLY: Interfaces and Adhesion II  
Morial Convention Center 214

11:15AM Y22.00001 Polymer monolayer - substrate adhesion strength  
MOSHE GOTTLIEB, HAIM DVIR, Ben-Gurion University — Polymer monolayers have been deposited on several chemically different solid substrates. The substrates ranged from hydrophobic to hydrophilic and from chemically inert to highly reactive. In addition few of the surfaces were also exposed to ionizing irradiation. The extent of surface coverage and surface topology were experimentally determined for the different surfaces and polymers. The adsorbed layer thickness was determined optically. The strength of polymer interaction with the substrate was investigated using contact-mode Atomic Force Microscopy. Typically, for each polymer a characteristic layer thickness was measured irrespective of the nature of the surface or strength of the polymer-surface adhesion. Adhesion strength was attributed mainly to van der Waals interactions with no indications of large scale covalent bonding between the polymer and the substrate. Hydrophobic interactions, surface topology, and initial conditions existing during film deposition seem to dominate the interaction between the polymer and the substrate.

11:27AM Y22.00002 Role of Interfacially Active Diblock Copolymers toward Controlling the Glass Transition of Thin Polymer Films  
HYUNJOON OH, PETER GREEN, University of Michigan, Ann Arbor — We show that small concentrations of polystyrene-b-poly(methylmethacrylate) (PS-b-PMMA) diblock copolymers significantly alter the thickness, h, dependence of the glass transition temperature as needed for the study of the glass transition in nanometer thin polymeric films. The glass transition in thin films was determined at well defined experimental time scales. No thickness dependency of the glass transition temperature was observed within the error limits - neither at constant frequency nor for the traces in the activation diagrams.

11:39AM Y22.00003 Weak interfaces for UV cure nanoimprint lithography  
FRANCES HOULE, ANN FORNO, IBM Almaden Research Center, EVA SIMONYI, IBM T.J. Watson Research Center, DOLORES MILLER, HOA TRUONG, IBM Almaden Research Center — Nanoimprint lithography using a photocurable organic resist provides a means of patterning substrates with a spatial resolution in the few nm range. The usefulness of the technique is limited by defect generation during template removal, which involves fracture at the interface between the template and the newly cured polymer. Although it is critical to have the lowest possible interfacial fracture toughness (Gc less than 0.1 Jm-2) to avoid cohesive failure in the polymer, there is little understanding on how to achieve this using reacting low viscosity resist fluids. Studies of debonding of a series of free-radical cured polyhedral silesquioxane crosslinker formulations containing selected reactive diluents from fluorosilane-coated quartz template materials will be described. At constant diluent fraction the storage modulus of cured resists follows trends in initial reaction rate, not diluent Tg. Adhesion is uncorrelated with both Tg and storage modulus. XPS studies of near-interface compositions indicate that component segregation within the resist fluid on contact with the template, prior to cure, plays a significant role in controlling the fracture process.
11:51AM Y22.00004 Spincoating of ultrathin chitosan films . CHRIS MURRAY, JOHN DUTCHER, University of Guelph — We have studied the spincoating of ultrathin chitosan films onto silicon wafer substrates from dilute solutions of chitosan dissolved in acetic acid solutions. This particular example of spincoating presents unique difficulties due to the non-volatility of the solvent, but also provides unique information since the spincoating process is slow enough to allow detailed measurements of the drying of the film. The resulting film thickness, as measured using ellipsometry, is a strong function of the relative humidity (RH) in the surrounding atmosphere, which can be easily controlled. By using a simple model for the dependence of film thickness on spin speed and RH, we obtain a measure of water uptake in chitosan films that can be compared with that estimated from sorption isotherms measured using ellipsometry.

12:03PM Y22.00005 Protein Diffusion at the Interface of Responsive Polymer Thin Films . SHENGQIN WANG, YINGXI ELAINE ZHU, Dept. of Chemical and Biomolecular Engineering, Univ. of Notre Dame, IN — Protein adhesion at polymer interfaces has been much explored, yet the interfacial friction is not. We employ fluorescence correlation spectroscopy (FCS) and single-molecule imaging to examine the translational dynamic processes of proteins at the responsive polymer interfaces, whose surface hydrophobicity and interfacial viscoelasticity are tunable experimentally. We focus on the dynamics of human serum albumin (HSA) and lubricin, a nutritious protein in synovial fluids, at the interface of responsive poly(N-isopropylacrylamide) (PNIPAM) brush layers. The effects of PNIPAM brush thickness, grafting density, and surface hydrophobicity on protein interfacial diffusivity are investigated. We observe the coupling of the local protein dynamics at the protein-PNIPAM interfaces with the interfacial viscoelasticity of PNIPAM brush thin films.

12:15PM Y22.00006 Structure and dynamics of molecules undergoing lubricated sliding . VIVEK PRABHU, SHUHUI KANG, KRISTOPHER LAVERY, NIST, KWANG-WOO CHOI, NIST, Intel Corp., WEN-LI WU, ERIC K. LIN, NIST — Polymer thin films are used as imaging layers for photolithography to define high spatial resolution features for the semiconductor industry. These chemically amplified photoresist materials, however, may be reaching their intrinsic limits as desired feature sizes approach macromolecular dimensions. A photocatalyzed reaction defines a chemical image which is subsequently resolved by dissolution in an aqueous base solution. A method to characterize the reaction-diffusion process was developed using infrared spectroscopy and tested by neutron reflectivity. We determine the thin film reaction kinetics, photocatalysis trapping behavior, and photoacid diffusivity by measuring the reaction kinetics. The temperature-dependent reaction rate and mechanism for observed pinning of the reaction-diffusion front will be discussed. These results predict the increase of the latent image formation which is a crucial step in photolithography resolution and fidelity.

12:27PM Y22.00007 Measurement advances to follow polymer thin film reaction-diffusion processes . LILIN HE, Clemson University — THUSITHA, ETAMPAWALA DVORA, PERAHIA Department of Chemistry, Clemson University, Clemson, SC 29634 JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM 87545 CHRISTOPHER J. CORNELIUS Sandia National Laboratories, MS 0886, Albuquerque, New Mexico 87185-0886 The penetration of solvent into a polymer that consists of incompatible groups is determined by the specific interactions with the guest molecule, where interfacial structure and dynamics of the polymer affect the onset of the process. The current work presents a neutron reflectometry study of the penetration of methanol into sulfonated polyphenylene thin films. The imonomer films were exposed to saturated deuterated methanol vapor and reflectometry patterns were recorded until equilibrium was reached. The process incorporates two stages where the vapors first wet the surface and then penetrate into the film. Significant swelling takes place as soon as the film is exposed to the vapors. Similar to previous studied in water, the onset diffusion is Fickian followed by an anomalous diffusion process. The entire process is faster than that observed for water.

12:39PM Y22.00008 Methanol Diffusion into Thin Ionomer Films: An in situ Study Using Neutron Reflectometry . LILIN HE, Clemson University — THUSITHA, ETAMPAWALA DVORA, PERAHIA Department of Chemistry, Clemson University, Clemson, SC 29634 JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, NM 87545 As the temperature increases, the polymer and its solvent will diffuse into each other, and the polymer film will expand and contract. The penetration of solvent into a polymer that consists of incompatible groups is determined by the specific interactions with the guest molecule, where interfacial structure and dynamics of the polymer affect the onset of the process. The current work presents a neutron reflectometry study of the penetration of methanol into sulfonated polyphenylene thin films. The imonomer films were exposed to saturated deuterated methanol vapor and reflectometry patterns were recorded until equilibrium was reached. The process incorporates two stages where the vapors first wet the surface and then penetrate into the film. Significant swelling takes place as soon as the film is exposed to the vapors. Similar to previous studied in water, the onset diffusion is Fickian followed by an anomalous diffusion process. The entire process however is faster than that observed for water.

12:51PM Y22.00009 Pattern formation in dewetting Nanoparticle/Polymer Bilayers . ALAN ESKER, RITUPARNA PAUL, UFUK KARABIYIK, MICHAEL SWIFT, JOHN HOTTLE, Virginia Tech — Comprised of inorganic cores and flexible organic coronae with 1 – 2 nm diameter monodisperse sizes, polyhedral oligomeric silsesquioxanes (POSS) are ideal model nanofillers. Our discovery that one POSS derivative, triisopropanol-POSS (TPP), can form Langmuir-Blodgett (LB) films on hydrophobic substrates, allows us to create thin film bilayers of precisely controlled thickness and architecture. Work with poly(t-butylacrylate) (PtBA)/TPP bilayers reveals a two-step dewetting mechanism in which the upper TPP layer dewets first, followed by the formation of isolated holes with intricate, fractal, nanofiller aggregates. Like the PtBA/TPP bilayers, poly(styrene) (PS)/TPP bilayers also undergo a two-step dewetting mechanism. However, the upper TPP layer initially forms cracks that may arise from mismatches in thermal expansion coefficients. These cracks then serve as nucleation sites for complete dewetting of the entire bilayer. Understanding the rich diversity of surface patterns that can be formed from relatively simple processes is a key feature of this work.

1:03PM Y22.00010 Case II diffusion and solvent-polymer films drying: a meso-scale model . DIDIER LONG, CNRS/Université de Paris Sud, MIREILLE SOUCHE, Université de Paris sud — This model is based on the fact that dynamics in liquids close to the glass transition is spatially heterogeneous [Ediger2000,Souche2007], with characteristic size 3 to 4nm in van der Waals liquids. Before considering large scale diffusion experiments, we consider first the evolution of the dynamics of a layer of thickness 3 to 4nm, submitted to an arbitrary time varying activity $a(t)$. This procedure allows in principle to calculate a constitutive relation for the dynamics of solvent-polymer mixtures, that can then be used for calculating the evolution of macroscopic samples in contact with a reservoir of solvent. We show how these constitutive relations allow for explaining case-II diffusion in glassy polymers and provide a physical interpretation for the parameters of the Thomas-Windle model. Regarding the process of film drying, we show that films up to 1 micrometer thick can be almost completely dried in an accessible experimental time, even at temperatures well below the polymer glass transition temperature. This is a consequence: 1- of the presence of the fast path 2- of the film being out equilibrium, and in a dynamical state which is much faster than the one it would have at equilibrium. When drying a thicker film, we show that a glassy crust may appear on the free surface, as has been shown experimentally. Ediger M.D., Annu. Rev. Chem., 51 (2000) 99; Souche M. and Long D., Europhys. Lett., 77 (2007) 48002.
1:15PM Y22.00011 Non solvent-induced dewetting of thin polymer films1. TONG-FEI SHI, LIN XU, LI-JIA AN — The dewetting of thin liquid films is important to various technological processes. Most of the studies on dewetting are through thermal dewetting, whereas solvent-induced dewetting has received very little attention. Generally the main difference between thermal dewetting and solvent-induced dewetting is that the cause of instability is the long-range force of van der Waals interactions in the thermal dewetting whereas it is the short-range force of polar interactions in the solvent-induced dewetting. In these reports on solvent-induced dewetting, nearly all solvents, which are chosen, can dissolve the polymers. However, few reports focus on the dewetting induced by non solvent, which cannot dissolve polymer. In this work, the process of non solvent-induced dewetting of thin polystyrene (PS) films on hydrophilic surfaces at room temperature has been studied by using water as a non solvent. It is observed that the process of non solvent-induced dewetting is greatly different from other previous dewetting processes. The PS film is in non-viscous state. A mechanism of non solvent-induced dewetting, different from other previous dewetting mechanisms, is deduced: penetration, replacement and coalescent.

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1:27PM Y22.00012 Mechanical Properties of Thin Polymer Films Studied by Atomic Force Microscopy, BLANDINE JEROME, LPMCN Lyon (F) & LBNL Berkeley, CHRISTIAN VIALLETON, LPMCN & MATEIS-INS Lyon (F), LAURENT CHAZEAU, MATEIS-INS Lyon (F), ELISABETH CHARLAIX, LPMCN Lyon (F) — Introducing inorganic nanoparticles into a polymer is known to modify the macroscopic mechanical properties of the material. This is often interpreted by assuming the presence of a polymer layer with different properties at the interface with the particles. There is however little direct information available on the mechanical properties of such an interfacial layer. We have used an Atomic Force Microscope (AFM) as a nano-indentor to probe the mechanical response of thin poly(styrene butadiene) random copolymers deposited on oxidized silicon wafers (model silica surface). Indentations were performed at different approach and retraction speeds at room temperature (polymer in the rubbery state) on films with thicknesses ranging from 40nm to 500nm. Approach and retraction curves obtained at high speeds are characteristic of the indentation of an elastic material with an adhesive tip/polymer contact. At low speeds, the adhesion forces dominate for low applied forces, while the elasticity of the polymer dominates the behaviour at high applied load. This allows us to separate the mechanical response of the polymer film from the tip-polymer adhesion that involves some dissipation taking place close to the contact line between the polymer free surface and the tip.

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1:39PM Y22.00013 Molecular Dynamics Simulations of Adhesion at Epoxy Interfaces, SARAH-JANE FRANKLAND, THOMAS CLANCY, National Institute of Aerospace, THOMAS GATES, NASA-LaRC — With composite materials becoming more prevalent as metal parts are being replaced on aircraft, adhesives are being developed for composite bonds which are suitable for the various thermal, mechanical and environmental changes that take place over the lifetime of the aircraft. The key molecular structure-property relationships that enable the chemical compatibility of the adhesive with the adherend can be identified with molecular dynamics simulation (MD). MD can assess the role of different chemical moieties in the adhesive, and their behavior in the presence or absence of solvents under different thermo-mechanical conditions. In the present work, MD simulations are used to calculate factors that affect the work of adhesion with and without solvent present. MD simulations are carried out at the interface between components of epoxy-based adhesives and composite adherends. The simulations utilize molecular models of networks which are representative of specific chemistries of the epoxy system. The simulations include both bulk and interface models of the components. The paper will present the simulation methodology, and the results for the work of adhesion.

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1:51PM Y22.00014 Interfacial Properties of Polydimethylsiloxane-Water Systems1, AHMED E. ISMAIL, GARY S. GREST, MARK J. STEVENS, Sandia National Labs, MESFIN TSIGE, Southern Illinois University at Carbondale, DAVID R. HEINE, Coming — Polydimethylsiloxane (PDMS) is a main constituent of silicone adhesives, which have a wide use as adhesives. Often these adhesives are used as sealants. The interaction between water and PDMS is of fundamental importance. To improve our understanding at the molecular level, we have performed molecular dynamics (MD) simulations of PDMS in the presence of water, with the long-term goal of studying how water molecules affect the mechanical behavior of PDMS at the surface. Knowledge of the basic interfacial properties of a multicomponent system, such as the surface tension, contact angle, and diffusion constant, are essential to obtain the proper dynamic behavior in a molecular simulation of adhesion and wetting processes. Explicit-atom simulations of 101 or more atoms were used to determine liquid-vapor surface tension and the contact angle for water on the surface of PDMS. We present results for the dependence of the surface tension on chain length and end-group functionality.

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1Supported by the NSFC (50503022) Programs and the Fund for Creative Research Groups (50621302), and subsidized by the Special Funds for National Basic Research Program of China (2003CB615600).

Friday, March 14, 2008 11:15AM - 1:15PM – Session Y23 DMP GMAG: Focus Session: Electronic Structure of Complex Oxides Morial Convention Center 215

11:15AM Y23.00001 Magnetic Moment Collapse-Driven Mott Transition in MnO1, JAN KUNES, University of Augsburg — Metal-insulator transition in strongly correlated electron systems has been one of the central themes of condensed matter physics for a few decades. In the simplest model system, the single band Hubbard model, the transition, which is still not completely understood, is driven by the ratio of the on-site repulsion to the bare bandwidth. Real materials with multiple bands offer possibility of alternative scenarios of the metal-insulator transition. In this talk we will present a numerical study of MnO under high pressure using combination of the standard bandstructure theory and modern many-body methods (dynamical mean-field theory). Our results reveal a close relationship between the high-spin to low-spin transition and metallization, which can be interpreted as the moment collapse driving the metallization. We find an inosstructural volume collapse of about 13% accompanying the transition. While the moment collapse, which is essentially an atomic effect, is obtained by most electronic structure methods, the metal-insulator transition can be described reliably only when dynamical correlations are taken into account. We find our results to compare very well to the available experimental data. In order to demonstrate the capability of the computational method PES and ARPES spectra obtained on the related NiO with and without hole doping will also be presented.

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1Supported by Alexander von Humboldt Foundation and DOE's Computational Materials Science Network.
11:51AM Y23.00002 Origin of magnetism in the Fe$_2$O$_3$–FeTiO$_3$ system from correlated band theory$^1$. ROSSITZA PENTCHEVA, HASAN SATAD NABI, University of Munich — The high remanent magnetization measured in ex-solutions of the canted antiferromagnet hematite (Fe$_2$O$_3$) and room-temperature paramagnet ilmenite (FeTiO$_3$) has recently received considerable attention not only in the geoscience community [1] but also for possible spintronics applications. To resolve the microscopic origin of magnetism in this system, we have performed density functional theory calculations, varying systematically the concentration, distribution, and charge state of Ti (Fe) in a hematite (ilmenite) host. We find that including electronic correlation within the LDA+U approach is decisive to obtain the correct ground state of the end members, α-Fe$_3^+$O$_2$ and Fe$^{2+}$Ti$^{4+}$O$_3$. In a single Ti layer in the hematite host, Ti is not inert as commonly assumed but plays an active role in compensating the charge mismatch at the interface and the emergence of magnetism and the preferred charge state is Ti$^{3+}$, Fe$^{4+}$. As soon as a thicker ilmenite-like block forms, the most favorable compensation mechanism is through Ti$^{2+}$ and a disproportionation in the Fe contact layer in Fe$^{2+}$, Fe$^{3+}$ giving theoretical evidence for the lanellar magnetism hypothesis [1]. The substitution of Ti (or Fe) in Fe$_2$O$_3$ (FeTiO$_3$) leads to impurity levels in the band gap and in some cases to half-metallic behavior.

$^1$Supported by the German Science Foundation (PE883/4-1) and ESF.

12:03PM Y23.00003 Electronic structure of Mn and Fe oxides, WALTER HARRISON, Stanford University — We present a clear, simple tight-binding representation of the electronic structure and cohesive energy (energy of atomization) of MnO, Mn$_2$O$_3$, and MnO$_2$, in which the formal charge states Mn$^{2+}$, Mn$^{3+}$, and Mn$^{4+}$, respectively, occur. It is based upon localized cluster orbitals for each Mn and its six oxygen neighbors. This approach is fundamentally different from local-density theory (or LDA+U), and perhaps diametrically opposite to Dynamical Mean Field Theory. Electronic states were calculated self-consistently using existing parameters [1], but it is found that the charge density is quite insensitive to charge state, so that the starting parameters are adequate. The cohesive energy per Mn is dominated by the transfer of two s electrons to oxygen p states, the same for all three compounds. The differing transfer of majority d electrons to oxygen p states, and the coupling between them, accounts for the observed variation in cohesion in the series. The same description applies to the perovskites, such as La$_2$Sr$_{1-x}$MnO$_3$, and can be used for FeO, Fe$_2$O$_3$ (and FeO$_2$); Because the formulation is local, it is equally applicable to impurities, defects and surfaces.


12:15PM Y23.00004 Configurational Electronic Entropy and the Phase Diagram of Mixed-Valence Oxides: The Cases of Li$_2$FePO$_4$ and Fe$_2$O$_3$$^4$. FEI ZHOU, Materials Science and Engineering, MIT, THOMAX MAXISCH, GERBRAND CEDER — We demonstrate that configurational electronic entropy, previously neglected, is a new factor controlling the final-temperature phase stability of mixed-valence oxides, in our case Li$_2$FePO$_4$. First-principles LDA+U calculations were performed on 245 Li$_2$FePO$_4$ structures with different lithium/vacancy and electron/hole distributions, and Monte Carlo simulations were used to determine the phase diagram based on a coupled cluster-expansion model. While transformations from low-T ordered or immiscible states are almost always driven by configurational disorder (i.e. random occupation of lattice sites by multiple species), in FePO$_4$–LiFePO$_4$ the formation of a solid solution is almost entirely driven by electronic, rather than ionic configurational entropy. We argue that such an electronic entropic mechanism, rather than an ionic one, may be relevant to most other mixed-valence systems. Details in Phys. Rev. Lett. 97, 155704 (2006). Recently we have studied the Verwey transition in magnetite Fe$_3$O$_4$. The configurational entropy of the $t_{2g}$ electrons on the iron B sub-lattice is found to lead to a first-order phase transition, although the mechanism is substantially more complicated than that Verwey originally proposed.

$^4$This work is supported by the DOE under Contract No. DE-FG02-96ER45571 and by the NSF MRSEC program under Contract No. DMR-0213282.

12:27PM Y23.00005 Can pristine semiconducting oxides be ferromagnetic? HAO HONG NGUYEN, Laboratoire LEMA, UMR 6157 CNRS, Université F. Rabelais, Tours, France, A. BARLA, CELLS-ALBA, Barcelona, Spain, J. SAKAI, Lab. LEMA, QUE HUONG NGUYEN, Marshall University, Huntington, WV 25701 — The recent finding of FM in HfO$_2$ thin films of Coey's group has urged us to re-judge the role of TM doping in introducing FM into semiconducting oxides. Our observation of FM in undoped TiO$_2$, HfO$_2$, In$_2$O$_3$, ZnO, and SnO$_2$ confirmed that magnetism is possible in pristine oxide thin films, and FM is likely due to oxygen vacancies. This assumption is confirmed by our XMCD measurement on TiO$_2$ films: The FM in TiO$_2$ films is indeed intrinsic, and stems from both O-2p and Ti-3d electrons. In semiconducting oxides, the origin of magnetism is not due to the doping, but oxygen vacancies/defects. A big issue is how to find a more appropriate model to explain the behavior of the mechanism. We propose a model based on an electronic structure calculation using the tight binding method in the confinement configuration. Vacancy sites in TiO$_2$, HfO$_2$, In$_2$O$_3$ films could create spin splitting and high spin state, so that the exchange interaction between the electrons surrounding the oxygen vacancy with the local field of symmetry could lead to a FM ground state. Calculations give the results of 3.18 $\mu_B$/vac for TiO$_2$, 3.05 $\mu_B$/vac for HfO$_2$ and 0.16 $\mu_B$/vac for In$_2$O$_3$. This model suggests that confinement effects play an important role in shaping up magnetic properties of low dimension systems.

12:39PM Y23.00006 Charge regulation via a negative feedback: transition metal atoms in semiconductors and insulators$^1$. HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO 80401 — Transition metal (TM) atoms in semiconductors and insulators produce energy levels in the band gap, whose occupation can be altered by shifting the Fermi level e.g. via doping. Changes in level occupation correspond to changes in the formal oxidation state. Such changes are associated with inward/outward lattice relaxations recorded as "ionic radii," different magnetic moments, and a core shift in x-ray photoemission. We show, via density-functional calculations within the plane-wave supercell method for TM atoms including Cr, Mn, Fe, and Co in the semiconductor hosts GaAs and Cu$_2$O, as well as in the ionic insulator host MgO, that changes in gap-level occupation result in only very small changes of charge on the TM atom itself. We show that this is due to an inherent negative feedback that regulates the TM charge via a TM–ligand rehybridization. Further, the inward/outward lattice relaxations and XPS core shifts, often associated with a change of the TM charge, in fact follow from the TM–ligand rehybridization, as the TM charge is kept unchanged via the inherent negative feedback.

$^1$Funded by DARPA under NREL contract No. DE-AC36-99GO10337.

12:51PM Y23.00007 Electronic Structure of Cubic Copper Monoxide, P.M. GRANT, W. SIEMONS, G. KOSTER, R.H. HAMMOND, T.H. GEBALLE, Stanford University — We report the calculation of the band structure and optical properties of the rocksalt form of copper monoxide. Although this particular crystal structure does not exist in bulk form for CuO, at least two groups, including ourselves, have succeeded in growing by "forced epitaxy," several atomic layers of cubic CuO on rocksalt proxy substrates such as MgO and STO. For our computation, we employed the DFT/LDA+U method known to give valid results for rocksalt NiO and FeO. Our results show cubic CuO, like these two materials, to be an antiferromagnetic Mott-Hubbard insulator whose band gap is primarily determined by charge transfer between filled O 2p bands and empty Cu 4s states, with localization of the Cu 3d hole by on-site coulomb repulsion frustrating what otherwise would be metallic behavior. We compare our results with NiO, FeO and the natural form of CuO found in the monoclinic mineral tenorite.
The spin-ladder compound Sr$_2$Cu$_2$O$_2$Cl$_2$ has a complex phase diagram including charge-density-wave order as well as unconventional superconductivity under high pressure. Due to its quasi-one-dimensional nature, fundamental questions about the high-$T_c$ cuprates might be more easily addressed in this context. However, due to the spatial proximity of neighboring ladders inter-ladder Coulomb repulsion as well as hopping between ladders might still be important. Using the functional renormalization group, we study a model of coupled Cu$_2$O$_2$ ladders. We investigate instabilities towards charge, spin, and pairing order as a function of hole doping, inter-ladder hopping, and interaction strength starting from experimentally relevant hopping parameter.\[1\]

Supported by DFG (F.S.) and NSF grant no. DMR-0605619

Session Y24 DCMP: Nanotube Devices and Applications

Friday, March 14, 2008 11:15AM - 2:15PM –

11:15AM Y24.00001 Self-Assembled, Self-Aligned Carbon Nanotube Thin Film Transistors

MICHAEL ENGEL, JOSHUA SMALL, YU-MING LIN, IBM T. J. Watson Research Center, ALEX GREEN, MARK HERSAM, Northwestern University, PHAEDON AVOURIS, IBM T. J. Watson Research Center — Carbon nanotube field-effect transistors (FETs) were fabricated and studied, and transistors (FETs) were fabricated and studied, and transistors in which there are no detectable secondary phases and the Curie temperature ($T_c$) is higher than 400 K. Single Mn$_x$Ge$_{1-x}$ nanowires could be the promising building blocks for both electrical and fundamental questions about the high-$T_c$ superconductors.

Carbon nanotubes used in this study have been purified and separated by their electronic structure, where the semiconducting tube percentage is as high as 99%, confirmed by both transport measurements on individual nanotubes and by optical absorption spectra. Through a simple self-assembly technique, we have produced aligned nanotube arrays. Thin film transistors based on these aligned nanotube arrays are fabricated with both back- and top-gate layouts, showing good switching performance and a high drive current. It is found that top-gated and back-gated devices exhibit distinct switching behaviors due to screening effects. Results on device channel length dependence will also be presented.


HOOTAN FARHAT, HYUNGBIN SON, YING FENG, MILDRED DRESSELHAUS, JING KONG, MIT — Heat dissipation is an important concern for nanoscale electronic devices. Freely suspended carbon nanotubes experience self heating during electron transport due to a lack dissipation channels for acoustic phonon\[1\]. Nanotubes lying on a SiO$_2$ substrate, however, are often assumed to be in good thermal contact with the underlying substrate \[2\]. In this work we show that there is substantial self-heating in nanotubes lying on a SiO$_2$ substrate. We use Raman spectroscopy to monitor the temperature of carbon nanotube field-effect transistors (FETs) as a function of the applied bias voltage. The temperature is determined from the shift in frequency and the broadening of the high energy Raman modes. Our results suggest that nanotubes FETs on a substrate can reach temperatures upwards of 700K before saturation. \[1\] Pop et al., PRL 95, 155505 (2005) \[2\] Lazzeri et al., PRB 73, 165419 (2006)

11:39AM Y24.00003 Gate-all-around carbon nanotube field-effect transistor

ZHIHONG CHEN, DAMON FARMER, IBM T.J. Watson Research Center, SHENG LIU, ROY GORDON, Department of Chemistry and Chemical Biology, Harvard University, PHAEDON AVOURIS, IBM T.J. Watson Research Center, JOERG APPIENZELLER, School of Electrical and Computer Engineering, Purdue University — The ultra-thin body of carbon nanotubes allows for aggressive channel length scaling while maintaining excellent gate control. In general, a gate-all-around (GAA) structure is expected to be the ideal geometry that maximizes electric field control in FETs. Combining the ultra-thin body of a carbon nanotube with a GAA device geometry is a natural choice for ultimate device design. In this talk, we demonstrate a gate-all-around single wall carbon nanotube field-effect transistor. This is the first successful experimental implementation of an off-chip gate and gate-dielectric assembly with subsequent deposition on a suitable substrate.

11:51AM Y24.00004 MnxGe1-x nanowires field-effect transistor for spintronics applications\[1\].

XINHAN HAN, MASAAKI OGAWA, MINSHEUNG WANG, KANG L. WANG, JUSTIN D. HOLMES, University of California, Los Angeles — Group IV Dilute Magnetic Semiconductors (DMS) materials attract much attention not only because of the potential for integration of DMSs with current COMS technology, but also the enhanced spin lifetime and coherent length due to small spin-orbit coupling and lattice inversion symmetry. On the other hand, nanowires are the versatile building blocks for the assembly of functional devices to do fundamental studies in nanoscale. Here we presents Mn$_x$Ge$_{1-x}$ (Mn ~ 0.5-1%) nanowires in which there are no detectable secondary phases and the Curie temperature ($T_c$) is higher than 400 K. Single Mn$_x$Ge$_{1-x}$ nanowire back gated field effect transistors (FETs) were fabricated and studied, and p-type depletion mode was observed with an on/off ratio of 10$^4$, threshold voltage of ~ 0.53 V, maximum transconductance of 0.2 $\mu$S, and subthreshold swing (SS) of 210 mV/decade. The mobility was estimated to be around 340 cm$^2$/Vs. These results show the high performance of our Mn$_x$Ge$_{1-x}$ nanowire FET, which indicates the Mn$_x$Ge$_{1-x}$ nanowires could be the promising building blocks for both electrical and spintronics devices.

\[1\] This work was in part supported by WIN, Western Institute of Nanoelectronics, funded by NRI (Nanoelectronics Research Initiative) and UC Discovery Grant

12:03PM Y24.00005 Transient Random Telegraph Signal in carbon nanotube field effect transistors\[1\], TSZ-WAH CHAN, BRIAN BURKE, KENNY EVANS, KEITH WILLIAMS, Department of Physics, University of Virginia — We have studied transient Random Telegraph Signal (RTS) induced in carbon nanotube-channel field effect transistors (FETs) by operating them at high bias. RTS arises from the population and depopulation of charge traps at specific energies that are scanned by sweeping the gate in a FET. At high bias, surface adsorbates/dopants interact with the SWNT and produce transient charge traps, which are manifest in the RTS signature. Transient RTS has been seen at temperatures from 200K up to room temperature. We speculate that RTS spectra could provide a characteristic signature of specific adsorbates or adducts on the nanotube channel. This capability is of interest not only for potential sensing technology but also provides a way to introduce controllable quantum interference resonances in the channel transport.

\[1\]Supported by DFG (F.S.) and NSF grant no. DMR-0605619
12:15PM Y24.00006 Large oscillating non-local voltage in multi-terminal single wall carbon nanotube devices\textsuperscript{1}, GUNNAR GUNNARSSON, University of Basel, JELENA TRBOVIC, University of Basel, CHRISTIAN SCHOENENBERGER, University of Basel, UNIVERSITY OF BASEL TEAM — Spin field-effect transistor has been recently realized in single wall carbon nanotube (SWCNT) devices contacted with NiPd alloy \cite{1}. In order to separate charge related effects from that of pure spin transport we measure a non-local voltage in SWCNTs by using a four-terminal structure. The four contacts divide the tube into three quantum dots (QD) which we control by the back-gate voltage $V_g$. We inject the current through the first QD by using excitation voltage of 200 $\mu$V and measure the non-local signal $V_{nl}$ across the third QD. We measure large oscillating non-local voltage as a function of $V_g$ with amplitude of $V_{nl} \sim 2\mu$V \cite{2}. While the classical resistor model can account for the negative sign of the non-local voltage its large amplitude means need deeper understanding. We discuss the origin of this large non-local signal and its effect on the non-local spin transport measurements in this type of devices. \cite{1} S. Sahoo, et al. Nature Phys. 1 99 (2005). \cite{2} G. Gunnarsson et al., arXiv:0710.0365v1.

\textsuperscript{1}This work has been supported by the Swiss Institute on Nanoscience, the Swiss National Science Foundation and the EU HYSWITCH project.

12:27PM Y24.00007 Probing the electrostatics of a metal-carbon nanotube Schottky diode using capacitive measurements, YU-CHIH TSENG, JEFFREY BOKOR, UC Berkeley — Capacitance-voltage measurement is a technique widely used to characterize metal-semiconductor contacts. We apply this technique to measure the capacitance-voltage across a p-type Schottky contact formed by titanium and a semiconducting carbon nanotube. Ohmic and Schottky contacts are made on the nanotube using palladium and titanium, respectively. The results agree qualitatively with simulations done using a Poisson-Schroedinger solver, considering only the electrostatics. We found additional frequency-dependent effects in the capacitance measurement that indicate the presence of electronic states arising from adsorbates or defects on the length of the nanotube.

12:39PM Y24.00008 Hypergolic fuel detection using Single Walled Nanotube Networks, SHARVIL DESAI, Dept. of Physics and Electrical and Computer Engg., University of Louisville, Louisville, KY, KAPILA HEWAPARAKRAMA, Dept. of Physics, University of Louisville, Louisville, KY, GAMINI SUMANASEKERA, Dept. of Physics and Electrical and Computer Engg., University of Louisville, Louisville, KY — Reliable and accurate detection of hypergolic fuels is vital to U. S. Missile Defense Agency. In this research a simple and highly sensitive SWNT network sensor was developed for real time monitoring of hydrazine leaks to ppm level concentrations. Upon exposure to hydrazine vapor, the resistance of n-type (after degassing) nanotubes is observed to decrease rapidly. The response time exhibits a linear dependence on the concentrations of the vapor. It was also found that the resistance of the sample can be recovered by pumping on the sample and exposing to UV light. The experimental results support chemical adsorption of hydrazine on SWNTs. Theoretical results of hydrazine-SWNT interaction \cite{1} are compared with the experimental observations. Results of similar study on ammonia, dimethyl hydrazine, and naphthalene will also be presented. \cite{1} Min Yu, C. S. Jayanthi, Shi-Yu Wu, APS 2008

12:51PM Y24.00009 Electrically Tunable Spin Polarization in a Carbon-Nanotube Spin Diode, CHRIS MERCHANT, NINA MARKOVIC, Johns Hopkins University — We have studied the current through a carbon nanotube quantum dot with one ferromagnetic and one normal-metal lead. For the values of gate voltage at which the normal lead is resonant with the single available non-degenerate energy level on the dot, we observe a pronounced decrease in the current for one bias direction. We show that this rectification is spin-dependent, and that it stems from the interplay between the spin accumulation and the Coulomb blockade on the quantum dot. Our results imply that the current is spin-polarized for one direction of the bias, and that the degree of spin polarization is fully and precisely tunable using the gate and bias voltages. As the operation of this spin diode does not require high magnetic fields or optics, it could be used as a building block for electrically controlled spintronic devices.

1:03PM Y24.00010 Detection of adsorbed gas atoms on suspended single-walled carbon nanotube micro-balances, ZENGHUI WANG, University of Washington, JIANG WEI, OSCAR VILCHES, DAVID COBDEN — Monolayers of gas atoms or molecules adsorbed on suspended single-walled carbon nanotubes offer the opportunity to study the phases and phase transitions of a unique low dimensional system. They are expected to resemble the well studied 2D monolayers on planar graphite, but with tight cylindrical boundary conditions imposed. The adsorbed density can be measured by using the nanotube itself as a vibrating microbalance, whose vibration amplitude is detected through the induced modulation of the conductance. We are initially studying the noble gases Ne, Kr and Xe, which are attractive for their simplicity and which show discontinuous phase transitions on 2D graphite that from basic considerations should be altered or suppressed as the dimensionality is reduced. We will also study oxygen monolayers, because oxygen has more complex 2D ordering on graphite, being magnetic and nonspherical, and because of the surprisingly large doping effect reported for oxygen on nanotubes which remains to be fully understood. We will survey the resonant behavior of a number of nanotube microbalances we have made, including examples with quality factor greater than 1000, and the damping effect of a gaseous environment. We will then report on our progress in detecting adsorbed layers and phase transitions in them.

1:15PM Y24.00011 Ab initio design of realistic nanotube sensors, ADALBERTO FAZZIO, ALEXANDRE ROCHA, MARIANA ROSSI, ANTONIO J.R. DA SILVA, Instituto de Física - USP Brazil — The understanding of the electronic transport properties of nanoscopic devices present tantalizing possibilities. It has been demonstrated that carbon nanotubes can be used as sensors for hazardous gases. Large scale computer simulations have an important role to play in predicting the transport properties of such systems. In order to do so one must take into account devices which are a few hundred nanometers in length and present defects randomly distributed along the structure. These defects act as binding sites for the molecules one wishes to detect. In this work we initially use density functional theory (DFT) to determine the most likely defects in highly nitrogen-doped carbon nanotubes, and to calculate the dissociation path of ammonia and hydrogen sulphide molecules onto these defects. Finally we use a combination of DFT and recursive Green’s functions techniques to first assemble and then calculate the electronic transport properties of nanotubes up to 200 nm in length and with defects randomly distributed along the structure. We demonstrate that these nanotubes present relatively large resistance changes even at low coverages which leads to highly sensitive devices. The result is a new paradigm in computer-aided sensor design, where one can simulate realistic sensors.

1:27PM Y24.00012 Utilizing Carbon Nanotubes for 1-D Mass Transport, GAVI BEGTRUP, A. ZETTL, University of California, Berkeley — Precision control of the size and placement of materials on the nanoscale creates many opportunities for customizable materials. Recent reports have shown that carbon nanotubes act as efficient one-dimensional mass transport platforms. We have designed nanotube devices on custom fabricated electron transparent substrates compatible with transmission electron microscopy in order to study mass transport mechanisms and applications in situ. Here we report the results of these studies.

1:39PM Y24.00013 Measurement of metal/carbon nanotube contact resistance by shortening contact length, CHUN LAN, DMITRI ZAKHAROV, RONALD REIFENBERGER, Birck Nanotechnology Center, Purdue University — Estimating the contact resistance to a minimum contact length of a nanotube interconnect to a nanoscale electronic device is a major challenge. In this study, we describe a novel experiment using a focused ion beam to sequentially shorten the contact length between a nanotube and an evaporated metallic film. We develop a theoretical model that relates the measured resistance change as a function of contact length to the intrinsic linear resistivity of the nanotube as well as the specific contact resistivity between the nanotube and the deposited metallic film. In this way, we arrive at an estimate for the optimal contact length of the metal film to the carbon nanotube. The results for Au and Ag contacts to multi-wall carbon nanotubes will be summarized. Our method is quite general and can be used to accurately determine the contact resistance of any metallic film to a wide variety of nanotubes and nanowires.
1:51PM Y24.00014 Bolometric Response of a Single-Wall Carbon Nanotube\textsuperscript{1}, DANIEL SANTAVICCA, JOEL CHUDOW, YAN YIN, MARKUS BRINK, ANTHONY ANNUNZIATA, LUIGI FRUNZIO, DANIEL PROBER, Dept. of Applied Physics, Yale Univ., ALAN TRUE, CHARLES SCHMUTTENMAER, Dept. of Chemistry, Yale Univ., MENINDER PUREWAL, YURI ZUEV, PHILIP KIM, Deps. of Physics and Applied Physics, Columbia Univ. — We report on the low temperature bolometric (thermal) rf response of individual metallic single-wall carbon nanotubes. This response is used to determine the thermal conductance of the nanotube. Previous work has demonstrated heterodyne mixing in individual carbon nanotubes using either an ac-driven I-V nonlinearity or a gate-modulated conductance. We distinguish between bolometric mixing and the response due to non-thermal electrical nonlinearities. These experiments are a precursor to proposed terahertz measurements of the frequency-dependent bolometric response of an individual single-wall nanotube.

\textsuperscript{1}This work is supported by NSF-CHE, NSF-DMR, and Yale University.

2:03PM Y24.00015 I-V transport measurements of a single unsupported MWCNT under various bending deformations\textsuperscript{1}, SUENNE KIM, Texas Materials Institute. University of Texas at Austin, JEEHOON KIM, MORGANN BERG, ALEX DE LOZANN\`{E}, Department of Physics, University of Texas at Austin — Using a home-made low-temperature high-vacuum probe setup we have obtained more details about the transport characteristics of multiwall carbon nanotubes (MWCNTs). We report our experimental studies on the improvement of the nanowelding between the CNTs and a metallic (W) probe tip in our SEM, which gives a clean and firm contact that satisfies for both electrical and mechanical requirements. We observe hysteresis of the I-V curves between bending and un-bending cycles, effective and efficient fabrication of junctions in the MWCNTs and their respective I-V characteristics, and the deformation-dependent saturation behaviors in the I-V curves of the MWCNTs. All these observations may be qualitatively understood using a simple phenomenological model for localizaion effects in the deformed hexagonal lattice of graphene.

\textsuperscript{1}Supported by Ilun foundation (SK) and NSF-DMR-0308575.

Friday, March 14, 2008 11:15AM - 2:03PM – Session Y25 DPOLY: Theory and Simulations III Morial Convention Center 217

11:15AM Y25.00001 Early Stage Crystallization in Isotactic Polypropylene: Influence of Nanofillers, RAHMI OZISIK, XIAOFENG CHEN, Rensselaer Polytechnic Institute, SANAT KUMAR, Columbia University, PHILLIP CHOI, University of Alberta — Formation of helices in isotactic polypropylene was studied using on-lattice, coarse-grained, Metropolis Monte Carlo simulations. Influence of polymer-particle interaction and particle size on polymer crystallization was studied by inserting isotropic particles into neat IPP melt. Results indicated that attractive interaction between polymer and particle plays a dominant role in the formation of helical structures. Repulsive interaction excludes polymer chains from the neighborhood of the surface and triggers crystallization transition earlier (at higher temperatures). Irrespective of the energy potential used, flat surface always influences the orientation of the helices to be parallel to the surface. Confinement effect was also investigated by changing the gallery spacing between two flat surfaces. Confinement significantly prohibits the growth of long helical structures but has no effect on the overall helicity as well as the ordering of helices.

11:27AM Y25.00002 Early Stage Crystallization in Isotactic Polypropylene: Influence of Substrate-Polymer Interaction and Confinement, XIAOFENG CHEN, RAHMI OZISIK, Rensselaer Polytechnic Institute, SANAT KUMAR, Columbia University, PHILLIP CHOI, University of Alberta — Formation of helices in isotactic polypropylene was studied using on-lattice, coarse-grained, Metropolis Monte Carlo simulations. Influence of polymer-substrate interaction on polymer crystallization was studied by placing IPP chains on a flat surface. Results indicated that attractive interaction between polymer and particle plays a dominant role in the formation of helical structures. Repulsive interaction excludes polymer chains from the neighborhood of the surface and triggers crystallization transition earlier (at higher temperatures). Irrespective of the energy potential used, flat surface always influences the orientation of the helices to be parallel to the surface. Confinement effect was also investigated by changing the gallery spacing between two flat surfaces. Confinement significantly prohibits the growth of long helical structures but has no effect on the overall helicity as well as the ordering of helices.

11:39AM Y25.00003 Growth, non-coalescence and assembly of water drops that form ordered arrays over evaporating polymer solutions, VIVEK SHARMA, School of Polymer, Textile and Fiber Engineering, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA 30332 — Breath figures are patterns formed, when cold solid or liquid substrates contact humid air. Typically, the condensed water drops exhibit a range of sizes, and their self-similar growth is marked by coalescence in late stages. But in the breath figures formed on evaporating polymer solutions exposed to the blast of humid air, non-coalescent drops grow and self-assemble into close packed arrays of nearly monodisperse drops. These drops evaporate away leaving an ordered array of air bubbles in polymer film. In this study, we elucidate the physics that drives nucleation, growth, non-coalescence and assembly of drops. We compute the growth kinetics of a droplet population under the mass and heat transport of water vapor that are intimately coupled with the corresponding fluxes of the evaporating solvent. We elucidate the role of solvent, polymer and air flow conditions and determine why the drops are non-sticky and why drops and pores are monodisperse.

11:51AM Y25.00004 Theory of competitive counterion adsorption on flexible polyelectrolytes: Divalent salts\textsuperscript{1}, ARINDAM KUNDAGRAMI, M. MUTHUKUMAR, Polymer Science and Engineering, University of Massachusetts Amherst — Counterion distribution around an isolated flexible polyelectrolyte in the presence of a divalent salt is evaluated using the adsorption model [M. Muthukumar, J. Chem. Phys. 120, 9343 (2004)] that considers temperature, salt concentration, and local dielectric heterogeneity as physical variables in the system. Self-consistent calculations of effective charge and size of polymer show that divalent counterions replace condensed monovalent counterions in competitive adsorption. The theory further predicts that at modest physical conditions, polymer charge is compensated and reversed with increasing divalent salt. Consequently, the polyelectrolyte collapses and reswells, respectively. Lower temperatures and higher degrees of dielectric heterogeneity enhance condensation of all species of ions. Complete diagram of states for the effective charge is calculated as functions of temperature and salt concentration. A simple theory of ion-bridging is also presented which predicts a first-order collapse of polyelectrolytes. The theoretical predictions are in agreement with generic results from experiments and simulations.

\textsuperscript{1}NSF, NIH, and MRSEC

12:03PM Y25.00005 Confinement free energy of flexible polyelectrolytes in spherical cavities, RAJEEV KUMAR, M. MUTHUKUMAR, UMASS, Amherst — A single flexible polyelectrolyte chain in a spherical cavity is analyzed using self-consistent field theory (SCFT) in the presence of solvent molecules and salt ions. It is found that the confinement of the chain leads to creation of a charge density wave along with the development of a potential difference across the centre of cavity and the surface. We have computed different energetic and entropic contributions to the free energy of the system. In particular, the role of wall-segment repulsive interactions and concentration fluctuations (at one loop level) in free energy has been explored. Results for the finite size corrections to free energy and osmotic pressure will be presented. Predictions about the effects of salt concentration, chain length, radius of the cavity, electrostatic interaction strength, degree of ionization and solvent quality will also be presented.
12:15PM Y25.00006 Simulation study of proton transport in ionomers\textsuperscript{1}. PHILIP TAYLOR, ELSHAD ALAHAYAROV, Case Western Reserve University — Coarse-grained molecular-dynamics simulations were used to study the morphological changes induced in a Naﬁon-like ionomer by the imposition of a strong electric ﬁeld. We observe that proton transport through this polymer electrolyte membrane is accompanied by morphological changes that include the formation of structures aligned along the direction of the applied ﬁeld. The polar head groups of the ionomer side chains assemble into clusters, which then form rod-like formations, and these cylindrical structures then assemble into a hexagonally ordered array aligned with the direction of current ﬂow. For dry ionomers, at current densities in excess of 1 A/cm\textsuperscript{2} these rod-like clusters undergo an inner micro-phase separation, in which distinct wire-like lines of sulfonate head groups are accompanied by similar wire-like alignments of bound protons. The clusters appear to be of two types. If there are two, four, or ﬁve lines of sulfonates then there is an equal number of lines of protons, but if there are three lines of sulfonates then they are accompanied by four lines of protons. Occasionally these lines of sulfonates and protons form a helical structure. Upon removal of the electric ﬁeld, the hexagonal array of rod-like structures remains, but the microphase separation disappears below the threshold current of 1 A/cm\textsuperscript{2}.

\textsuperscript{1}Work supported by DOE Grant DE-FG02-05ER46244.

12:27PM Y25.00007 Polymer capture by electro-osmotic ﬂow of oppositely charged nanofluids. CHU TAI ANDREW WONG, M. MUTHUKUMAR, Department of Polymer Science and Engineering, University of Massachusetts Amherst — We have addressed theoretically the hydrodynamic effect on the translocation of DNA through nanopores. We consider the cases of nanopore surface charge being opposite to the charge of the translocating polymer. We show that, because of the high electric ﬁeld across the nanopore in DNA translocation experiments, electro-osmotic ﬂow is able to create an adsorbing region comparable to the size of the polymer around the nanopore. Within this capturing region, the velocity gradient of the ﬂuid ﬂow is high enough for the polymer to undergo coil-stretch transition. The stretched conformation reduces the entropic barrier of translocation. The diffusion limited translocation rate is found to be proportional to the applied voltage. In our theory, many experimental variables (electric ﬁeld, surface potential, pore radius, dielectric constant, temperature, and salt concentration) appear through a single universal parameter. We have made quantitative predictions on the size of the adsorption region near the pore for the polymer and on the rate of translocation.

12:39PM Y25.00008 Depletion interaction and effect of polydispersity in non-adsorbing polymer solutions\textsuperscript{1}. DADONG YAN, SHUANG YANG, C.C. HAN, State Key Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, China, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada — The depletion effect between two spherical colloidal particles in non-adsorbing polymer solutions is investigated using the self-consistent ﬁeld theory. The density distributions of polymer segments, the depleted amount and depletion potential are calculated numerically in bi-spherical coordinates. The effects of chain length, bulk concentration, and solvency are also investigated for the dilute regime, semidilute regime and high concentration. Also, the effect of polymer polydispersity on the depletion interaction between two plates immersed in a non-adsorbing polymer solution with Schulz molecular weight distribution is studied within self-consistent-ﬁeld theory. For the case of two large spheres the Derjaguin approximation is used to study the effect of polydispersity.

\textsuperscript{1}NSFC Major Project No.20490220.

12:51PM Y25.00009 Unimolecular spreading of a molecular brush on adsorbing surface. EKATERINA ZHULINA, Institute of Macromolecular Compounds 199004 St. Petersburg Russia, SERGEY PANYUKOV, Lebedev Physics Institute 117924 Moscow Russia, MICHAEL RUBINSTEIN, University of North Carolina Chapel Hill NC 27599 USA — Using scaling concepts and the analytical self-consistent-ﬁeld theory we explore different conformations of a molecular brush on a planar substrate in nonsolvent environment (air-solid interface). The relationship between architecture and stress in adsorbed macromolecule is determined in terms of spreading parameter, grafting density and degree of polymerization of the side chains. A novel tentlike shape of molecular cross-section as well as rectangular and combined (tentlike + rectangular) conformations are predicted and examined. We demonstrate that strong adsorption of densely branched macromolecules on a planar substrate can lead to stress in molecular backbone sufficient to break covalent bonds.

1:03PM Y25.00010 Effect of chain stiffness on structural and thermodynamic properties of polymer melts. JUTTA LUETTMER-STRATHMANN, University of Akron — Static and dynamic properties of polymers are affected by the stiffness of the chains. In this work, we investigate structural and thermodynamic properties of a lattice model for semiflexible polymer chains. The model is an extension of Shaffer's bond-ﬂuctuation model\textsuperscript{1} and includes attractive interactions between monomers and an adjustable bending penalty that determines the Kuhn segment length. For isolated chains, a competition between monomer-monomer interactions and bending penalties determines the chain conformations at low temperatures. For dense melts, packing effects play an important role in the structure and thermodynamics of the polymeric liquid. In order to investigate static properties as a function of temperature and chain stiffness, we perform Wang-Landau type simulations and construct densities of states over the two-dimensional state space of monomer-monomer and bending contributions to the internal energy. In addition, we present ﬁrst results from an algorithm for equation-of-state effects in lattice models.


1:15PM Y25.00011 Ameba-like diffusion in two-dimensional polymer melts: how critical exponents determine the structural relaxation. TORSTEN KREER, HENDRIK MEYER, JOERG BASCHNAGEL, Institut Charles Sadron, 6 rue Boussingault, 67083 Strasbourg, France — By means of numerical investigations we demonstrate that the structural relaxation of linear polymers in two dimensional (space-filling) melts is characterized by ameba-like diffusion, where the chains relax via frictional dissipation at their interfacial contact lines. The characteristic diffusion exponents determine the length scale, which does not exist in three dimensions. We show how this length scale follows from the critical exponents, which hence characterize not only the static but also the dynamic properties of the melt. Our data is in agreement with recent theoretical predictions, concerning the time-dependence of single-monomer mean-square displacements and the scaling of concomitant relaxation times with the degree of polymerization. For the latter we demonstrate a density crossover-scaling as an additional test for ameba-like relaxation. We compare our results to the conceptually different Rouse model, which predicts numerically close exponents. Our data can clearly rule out the classical picture as the relevant relaxation mechanism in two-dimensional polymer melts.

1:27PM Y25.00012 Connections between static and dynamic properties of atheral polymer melts: a Monte Carlo simulation study. NENAD STOJILJOVIC, Physics Department, John Carroll University, JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron — The motion of individual chains in polymer melts and blends is governed by local friction and entanglement effects. In simulations and experiments it can be difﬁcult to separate these effects since both local friction coefﬁcients and entanglement lengths depend on the thermodynamic state and the chain structure and since many systems display neither ideal Rouse nor fully entangled dynamics. In this work, we investigate local and chain dynamics of atheral polymer melts with Monte Carlo simulations of two versions of Shaffer's bond-ﬂuctuation model\textsuperscript{1}. S. Shaffer, J. Chem. Phys. 101, 4005 (1994). In the ﬁrst version, bonds are allowed to cross each other with the result that the chains do not entangle; in the second, bond crossings are prohibited and entanglement effects become apparent. Since both versions of the model have very similar static properties, local friction and entanglement effects can be separated. With simulations for a range of densities and chain lengths, we investigate connections between static and dynamic properties, in particular, scaling with the packing length and the size of the moving segment responsible for local friction.
1:39PM Y25.00013 Thermodynamic modeling of melt deformation.1,  J.P. IBAR, Universite de Pau, Pau 64013 France — In current tube models, the chain is the focus of interest; it is the statistical system. For entangled chains, part of the chain (of molecular weight M) becomes the system. In the statistical model of this paper, systems are sets of conformers coherently interactive, where interactive coupling is defined with respect to 2 types of interaction between conformers, covalent or intermolecular. The duality is explained by a new statistics, a crossed-statistics, which calculates the conformational state of all conformers, not just whether they are cis, gauche or trans, but also whether they are either covalently or inter-molecularly bonded. Entanglements manifestation result from a disturbance of the crossed-statistics by the increase of the number of covalently bonded conformers resulting in thermodynamically stable dual phases. The deformation of a statistical system results from a change of the conformation population between the flexed and trans conformations in the direction of the imposed macroscopic field vector. Shear or elongational flow mechanisms differ for the amount played by diffusion in feeding the deformed systems with undeformed (or relaxed) conformers to minimize the total energy required to accommodate the macroscopic deformation. Strain, strain rate and temperature determine how many systems are deformed and to what extent.

1Work under Fulbright Fellowship Award

1:51PM Y25.00014 Can a material clock based model describe highly non-linear creep?1, GRIGORI MEDVEDEV, JAMES CARUTHERS, Purdue University — Most constitutive models developed to date assume that the non-linear behavior observed in glassy polymers is due to a deformation dependent material clock, where the challenge is to find the correct functional form of how the rate of relaxation depends upon structural variables. A two order-of-magnitude change in mobility upon deformation has been observed experimentally [1], confirming that a material clock is a necessary component of any constitutive description. A non-linear viscoelastic constitutive theory [2], where the clock is configurational energy based, captures with a single parameter a wide variety of phenomena, including yield, stress/ volume/ enthalpy relaxation, and physical aging. The model is also successful in describing linear creep and recovery; however, it fails dramatically in case of highly non-linear creep in the glass transition region. No change in the functional form of the material clock can significantly improve the prediction of the model for non-linear creep. We postulate that spatial dynamic heterogeneity of glassy materials, which is well established experimentally, must be incorporated into the constitutive model in order to describe non-linear creep. [1] Ediger, et al., APS Meeting - Denver, CO March, 2007. [2] Caruthers, et al., Polymer, 45, 4577-4597, 2004.

Friday, March 14, 2008 11:15AM - 2:15PM –
Session Y27 GMAG: Focus Session: Kagome Magnets Morial Convention Center 219

11:15AM Y27.00001 Magnetic Diffuse Scattering in the Frustrated Kagome Antiferromagnet YBaCoO$_3$ — PASCAL MANUEL, LAURENT CHAPON, PAOLO RADAELLI, ISIS Facility, Rutherford Appleton Laboratory, JOHN MITCHELL, HONG ZHENG, Materials Science Division, Argonne National Laboratory, 9700 S. Cass Ave, Argonne IL 60439 — Cobalt oxides of composition RBaCo$_2$O$_7$ (R=Y, Tb-Lu) crystallize with a lattice structure topologically related to that of the pyrochlore. Considering only the magnetic transition metal sublattice, R-114 appears as Kagome sheets linked by triangular layers and is therefore expected to provide a new materials class for exploring geometric magnetic frustration. We have recently shown that stoichiometric R-114 compound orders antiferromagnetically into a long-range ordered (LRO) structure with features common to the $\sqrt{3} \times \sqrt{3}$ negative chirality spin arrangements often found in Kagome net systems. In contrast, small excesses of O added to the system, as little as 0.1, destroys this LRO state. To explore the nature of the frustrated magnetism in this novel system, we have measured magnetic diffuse scattering on YBaCo$_3$O$_7$ and YBaCo$_2$O$_7$-$\delta$ single crystals at the ISIS facility. Large maps of reciprocal space in several planes have been recorded showing a very structured diffuse scattering. The data compared to models obtained by the Monte-Carlo method using the metropolis algorithm, reveal the exact nature of the disordered ground state in this new class of frustrated magnets.

11:27AM Y27.00002 $^{65}$Cu, $^{35}$Cl, and $^1H$ NMR in the S=1/2 Kagomé Lattice ZnCu$_7$(OH)$_6$Cl$_2$ — TAKASHI IMAI, Dept. of Physics, McMaster University, Canada, E.A. NYTKOC, B.M. BARTLETT, M.P. SHORES, D.G. NOCERA, Dept. of Chemistry, M.I.T. — ZnCu$_7$(OH)$_6$Cl$_2$ (S=1/2) is a promising new candidate for an ideal Kagomé Heisenberg antiferromagnet, because there is no magnetic phase transition down to ~50 mK. We investigated its local magnetic and lattice environments with NMR techniques (ArXiv:cond-mat/0703141). From $^{35}$Cl Knight shift data, we demonstrate that the intrinsic spin susceptibility follows a Curie-Weiss law down to ~0.2T, then decreases toward T = 0. Comparison of $^1H$ and $^{35}Cl$ spin-lattice relaxation rate 1/T$_{1}$ evidences for slow freezing of the lattice near ~50 K, presumably associated with OH bonds. Spin dynamics near T = 0 obey a power-law behavior in the presence of high magnetic fields.

11:39AM Y27.00003 Theory of Collinear ordering on the Kagome Lattice of Zn-parataramite$^3$ — LARS FRITZ, Harvard University, MICHAEL LAWLER, YONG-BAEK KIM, University of Toronto, SUBIR SACHDEV, Harvard University — We present a theory of the collinearly ordered phase discovered in a recent neutron scattering experiment [1] on Zn-paratacamite, Zn$_3$Cu$_4$(OH)$_6$Cl$_2$, at small x. Zn-parataramite has been considered as an excellent model system for the kagome lattice of spin-1/2 moments with antiferromagnetic exchange interactions. We studied both the classical and quantum Heisenberg models on the distorted kagome lattice appropriate for Zn-parataramite with small x. Our theory naturally explains the emergence of the valence bond solid phase. We suggest future inelastic neutron and elastic X-ray scattering experiments that can test our predictions.

$^3$NSF grant No. DMR 0537077; DFG FR 2627/1-1 ; KRF-2005-070-C00044

11:51AM Y27.00004 Theory of the Valence-Bond-Solid Phase on the Kagome Lattice of Zn-parataramite — MICHAEL LAWLER, Harvard University of Toronto, LARS FRITZ, Harvard University, YONG-BAEK KIM, University of Toronto, SUBIR SACHDEV, Harvard University — We present a theory of the valence-bond solid phase discovered in a recent neutron scattering experiment [1] on Zn-paratacamite, Zn$_3$Cu$_4$(OH)$_6$Cl$_2$, at small x. A theory of the Neel phase also discovered in this experiment will be presented in a related contributed talk. Zn-parataramite has been considered as an excellent model system for the kagome lattice of spin-1/2 moments with antiferromagnetic exchange interactions. We study both the classical and quantum Heisenberg models on the distorted kagome lattice appropriate for Zn-parataramite with small x. Our theory naturally explains the emergence of the valence bond solid phase. We suggest future inelastic neutron and elastic X-ray scattering experiments that can test our predictions.

$^1$S.-H. Lee et al., Nature Materials, 6, 853

$^3$This work was supported by grant #CTS-0506840 from the National Science Foundation.
12:03PM Y27.00005 New natural spin-1/2 kagomé systems — kapellansite Cu$_2$Zn(OH)$_6$Cl$_2$ and haydeeite Cu$_2$Mg(OH)$_6$Cl$_2$, OLEG JANSON, HELGE ROSNER, Max-Planck-Institute for Chemical Physics of Solids Dresden, Germany — New natural spin-1/2 systems with kagomé layers — kapellansite Cu$_2$Zn(OH)$_6$Cl$_2$ and haydeeite Cu$_2$Mg(OH)$_6$Cl$_2$ — are studied by full potential density functional calculations using the fpblo.00-24 code. The band structure, obtained by a paramagnetic calculation, was used to solve a tight-binding model. The transfer integrals were mapped subsequently to a Hubbard model and to a Heisenberg model, giving an estimate for the antiferromagnetic (AF) exchange. The total exchange, containing AF and ferromagnetic (FM) parts, was derived from LSDA + U supercell calculations. As the main result, we find that in both compounds only two exchange integrals are relevant: the nearest neighbour exchange $J_1$ and the interaction $J_2$ along the diagonals of the Cu$^{2+}$-hexagons. Surprisingly, the size of these integrals depends strongly on the O—H bond length which was therefor optimized with respect to the total energy, resulting in about 1 Å for both compounds. Using the optimized O—H bond length, we find $J_1 > J_2$ in kapellansite and $J_1 < J_2$ in haydeeite. According to our results, kapellansite can be described as a modified kagomé lattice, while interpenetrating chains should be considered for haydeeite. Our results should encourage new experimental studies of these interesting materials.

12:15PM Y27.00006 Classical antiferromagnet on a hyper-kagome lattice, JOHN HOPKINSON, Brandon University, SERGEI ISAKOV, ETH-Zurich, HAE-YOUNG KEE, YONG BAEK KIM, University of Toronto — Motivated by recent experiments on Na$_2$IrO$_4$ [Y. Okamoto et al., Phys. Rev. Lett. 99, 167402 (2007)], we study the classical antiferromagnet on a frustrated three-dimensional lattice obtained by selectively removing one of four sites in each tetrahedron of the pyrochlore lattice. This “hyper-kagome” lattice consists of corner-sharing triangles. We present (J. Hopkinson et al., Phys. Rev. Lett. 99, 037201 (2007)) the results of large-$N$ mean field theory and Monte Carlo computations on $O(N)$ classical spin models. We find the classical ground states to be highly degenerate. Nonetheless, at low temperatures, nematic order emerges via “order by disorder” in the Heisenberg model ($N=3$), representing the dominance of coplanar spin configurations. Above this transition, the spin-spin correlations show a dipolar form which can be understood to arise from a generalized “Gauss” law constraint. The relevance of these results to ongoing neutron scattering experiments will be discussed.

12:27PM Y27.00007 Tuning of the spin liquid ground state in the kagome system Pr$_3$Ga$_2$XO$_{14}$,‡ C. R. WIEBE, H. D. ZHOU, Y.-J. JO, M. A. CASTELLANO, L. BALICAS, M. J. CASE, Y. QIU, J. R. D. COPLEY, V. RAMACHANDRAN, N. S. DALAL, J. S. GARDNER — We report on the single crystal growth of the series of kagome oxides Pr$_3$Ga$_2$XO$_{14}$ ($X$ = Si, Ti, Ge, and Sn). The material Pr$_3$Ga$_2$SiO$_{14}$ has near neighbor antiferromagnetic interactions between the Pr spins ($\theta$ = -2.3 K), but there is no long range order down to 0.035 mK ($f$ = 66). The presence of 2D low energy spin excitations results in a strong $T^2$ component to the specific heat typical of other kagome systems such as SCGO. By tuning the size of the lattice through substitution on the Si site, one can adjust the exchange between the spins in a regular fashion. Our data shows a systematic decrease in the amplitude of the $T^2$ component of the specific heat as the magnetic exchange becomes weaker through Ti and Ge substitution. In the case of Sn doping, the system orders as the dipolar interactions dominate over the weak antiferromagnetic exchange. To our knowledge, this is the first example of a tunable spin liquid kagome system.

‡Supported by the NSF (DMR-0084173, DMR-0454672), the EIEG program, and the state of Florida

12:39PM Y27.00008 Thermodynamics of Ising Spins on the Triangular Kagome Lattice,‡ YEN LEE LOH, DAOXIN YAO, ERICA W. CARLSON, Purdue University — In the compounds Cu$_2$X$_2$O$_{16}$ ($X$=Zn, Cd, Ge, Mn) and Cu$_2$GeO$_3$, the Cu spins form a fascinating and unique pattern called a triangular kagome lattice (TKL). We present a detailed study of Ising spins on such a lattice using exact methods and Monte Carlo simulation. We calculate the free energy, internal energy, specific heat, entropy, sublattice magnetizations, and susceptibility, and we find a rich phase diagram as a function of coupling constants, temperature, and applied magnetic field. In the frustrated regime at $T=0$, the system effectively decouples into independent states of freedom, giving residual entropy $S_0 = \frac{1}{2} \ln 72$ per spin and correlation length $\xi = 0$ — an interesting contrast with the triangular and kagome lattice Ising models. Applying a field induces a critical phase (related to the honeycomb lattice dimer model) that has irrational $1/\sqrt{2}$ correlations that should be detectable by neutron scattering. 1

We gratefully acknowledge support from Research Corporation.

12:51PM Y27.00009 Spin Triplet Excitations of the Heisenberg Antiferromagnet on the Kagome Lattice,‡ KWON PARK, Korea Institute for Advanced Study, BOHM-JUNG YANG, Seoul National University, YONG BAEK KIM, University of Toronto, JAEJUN YU, Seoul National University — The Kagome lattice Heisenberg antiferromagnet is one of the most frustrated spin systems in two dimensions, with many generated various theoretical proposals for the ground state. While recent experiments strongly suggest that the ground state is not magnetically ordered, identification of the true ground state remains highly controversial. Possible candidate phases include various spin liquids and a valence bond solid, particularly with a 36-site unit cell. It is therefore important to theoretically explore decisive properties of the candidate ground states which can be directly compared with experiments. To this end, we investigate the low-energy spin triplet excitations of the valence bond solid state with a 36-site unit cell, which are gapped in contrast to spin singlet excitations. Implications to future experiments are discussed.

‡Supported by the NSF (DMR-0084173, DMR-0454672), the EIEG program, and the state of Florida

1:03PM Y27.00010 Multiple magnetic phases in the frustrated spin-dimer compound Ba$_2$Mn$_2$O$_4$,‡ E. C. SAMULON, Stanford University, Y.-J. JO, National High Magnetic Field Laboratory, P. SENGUPTA, Los Alamos National Laboratory, G. M. SCHMIEDEHOFF, Occidental College, C. D. BATISTA, M. JAIME, Los Alamos National Laboratory, L. BALICAS, National High Magnetic Field Laboratory, I. R. FISHER, Stanford University — Ba$_2$Mn$_2$O$_4$ is a spin-dimer compound based on S=1 3d$^3$ Mn$^{3+}$ ions on a triangular lattice. Antiferromagnetic intradimer exchange leads to a singlet ground state in zero-field. Here we present the first results of thermodynamic measurements for single crystals probing the high-field ordered states of this material. Specific heat, magnetocaloric effect, torque magnetometry and magnetotension measurements were performed in magnetic fields up to 32 T and temperatures down to 20 mK. These measurements reveal the presence of multiple ordered states for fields above $H_c1 \sim 8$ T. Both single-ion anisotropy and geometric frustration play crucial roles in determining the phase diagram.

‡Work at Stanford is supported by the NSF under grant DMR 0705087

1:15PM Y27.00011 135,137$^+$Ba NMR study of Ba$_3$Mn$_2$O$_7$. STEVE SUH, W.G. CLARK, GUOQING WU, S.E. BROWN, UCLA, E.C. SAMULON, I.R. FISHER, Stanford, C.D. BATISTA, LANL, A.P. REYES, P. KUHNS, L.L. LUMATA, NHMFL, Tallahassee — We report results from 135,137$^+$Ba NMR spectroscopy and relaxation rate ($1/T_1$) measurements in single crystal Ba$_3$Mn$_2$O$_7$, an S=1 dimer system with a singlet ground state. Thermodynamic measurements have shown it has multiple field-induced phase transitions for fields exceeding a critical field $H_c1 \sim 90$ K and varying with field orientation. We have evaluated the hyperfine couplings and electric field gradients in the normal phase for one of the two inequivalent Ba sites, and find a significant anisotropic component to the hyperfine coupling. Measurements of $1/T_1$ made at fixed fields down to temperatures $T < 0.4$ K are consistent with critical behavior in the vicinity of $H_c1$. However, lower temperatures are needed to clarify the universality class. Goals for upcoming experiments include a determination of the spectrum in the low-symmetry phases and an evaluation of $1/T_1$ for $T < 0.4$ K. This work is supported at UCLA by NSF Grants 0520552 (SEB), DMR-00334869 (WGC), Stanford by DMR-0134613 (IRF), and NHMFL by 0084173 and the State of Florida.
3+ evolution: (1) suppressed structural distortion leading to geometric frustration, and (2) the formation of $S=0$ Co centers that can break magnetic exchange pathways. The pitch of the spiral is substantially larger than when the chains are coupled in an unfrustrated square-lattice geometry. The CAF phase does not appear to be stabilized for any value of $J_1/J_2$ for the spin-one model.

1:39PM Y27.00013 Spin order and excitations of a model triangular antiferromagnet, WEI BAO, Los Alamos National Lab., YINGMING QIU, NIST, YINXIA WANG, KUO LI, JIANGHUA LIN, Peking University, ROSS ERWIN, NIST — The triangular antiferromagnet is a model system sittinguate close to the boundary between a three-sublattice order and a quantum-liquid state, due to delicate balance among magnetic interaction, quantum fluctuations and geometrical frustration. The unique topology of the non-collinear three-sublattice order has profound consequences in finite-temperature phase-transitions and spin excitations, which are not yet fully understood. Experimental investigation on such issues has been impeded by imperfect materials which fail to represent the theoretical model at low temperatures. Here we show by neutron scattering that the three-sublattice order in the exceptional new material La$_2$Ca$_2$MnO$_6$ remains two-dimensional down to 40 mK. The order parameter and critical spin fluctuations suggest a phase transition at 3.8 K, but the in-plane correlation length becomes resolution-limited only below 1.8 K. While the spin-wave cone at low energy and the softening of high-energy modes in current theories are supported by our observations, measured spectral intensity above the upper energy limit of spin-waves distribution and a pseudogap developing below 1.8 K are not anticipated.

3 Works supported by the US DOE, NNSF of China, and NSF.

Friday, March 14, 2008 11:15AM - 1:27PM — Session Y28 DCMP: Superlattices and Nanostructures: Electronic Properties III — Morial Convention Center 220

11:15AM Y28.00001 Layer interdependence of transport in an undoped electron-hole bilayer, CHRISTIAN MAROTH, JOHN SEAMONS, JOHN RENO, MIKE LILLY, Sandia National Lab — Recently interest in the layer interdependence of a bilayer’s transport has emerged. To examine this dependence the layer transport properties in an undoped electron-hole bilayer (uEHBL) device were measured as a function of density, inter-layer electric field and temperature. The uEHBL device consisted of a tunable, independently-contacted two-dimensional electron gas (2DEG) and two-dimensional hole gas (2DHG) in direct GaAs quantum wells separated by a 30 nm Al$_x$Ga$_{1-x}$As barrier. At $T = 0.3$ K, the 2DHG mobility increased with increasing 2DEG density, while the opposite effect was not observed. Decreasing the inter-layer electric field also increased 2DHG mobility without affecting the 2DEG mobility. This also decreased 2DHG Coulomb drag suggesting the inter-layer separation was increased. Distinct temperature dependencies were also measured for each layer’s density and resistivity.

3 This work was supported by the Div. of Mat. Sci. and Eng., Office of Basic Energy Sciences, U.S. Dept. of Energy. Sandia is operated by Sandia Corp., a Lockheed Martin Company, for the U.S. Dept. of Energy under Contract No. DE-AC04-94AL85000.

11:27AM Y28.00002 Electronic doping in heterostructures of strongly correlated materials, IVAN GONZALEZ, Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN, ROGER G. MELKÓ, Department of Physics and Astronomy, University of California, Davis. — We have performed inelastic neutron scattering measurements on a single crystal sample of YBaCo$_4$O$_{10+δ}$, triangular lattice $(J_1 = 0)$, triangular lattice $(J_1 = J_2)$ and decoupled one dimensional linear chains $(J_2 = 0)$. Results are obtained by means of linked-cluster series expansions around the collinear antiferromagnetic phase (CAF) and the non collinear antiferromagnetic phase (NCAF), also known as the spiral phase. For the spin-half model, both phases can be stabilized within our calculations for small $J_2$. However, the NCAF phase always appears to have a lower energy. The pitch of the spiral is substantially renormalized from the classical values. For the spin-one model, we find a transition from the Haldane gap phase to the NCAF phase as a function of $J_1/J_2$. Interchain coupling required for this transition is more than a factor of 30 larger than when the chains are coupled in an unfrustrated square-lattice geometry. The CAF phase does not appear to be stabilized for any value of $J_1/J_2$ for the spin-one model.
11:51AM Y28.00004 Electronic states in magnetic quantum dots and quantum-dot molecules: Coulomb interaction effects and spontaneous symmetry breaking, ALEXANDER GOVOROV, Ohio University, WEI ZHANG, Ohio University & Institute of Applied Physics and Computational Mathematics, Beijing, China — We investigate theoretically few-electron states in semi-magnetic quantum dots and quantum-dot molecules [1,2]. A double quantum-dot system made of diluted magnetic semiconductor behaves unlike the usual molecules. In a semiconductor double quantum dot or in a diatomic molecule, the ground state of a single carrier is described by a symmetric orbital. In a magnetic material molecule, new ground states with broken symmetry can appear due to the competition between the tunneling and magnetic polaron energy. With decreasing temperature, the ground state changes from the normal symmetric state to a state with spontaneously broken symmetry. Interestingly, the symmetry of a magnetic molecule is recovered at very low temperatures. A magnetic double quantum dot with broken-symmetry phases can be used as a voltage-controlled nanoscale memory cell. [1] A. O. Govorov, Phys. Rev. B 72, 075359 (2005). [2] W. Zhang, T. Dong, and A. O. Govorov, Phys. Rev. B 76, 075319 (2007).

12:03PM Y28.00005 The Kondo Effect and Rashba Spin-Orbit Coupling, JUSTIN MALECKI, University of British Columbia — We present the results of a study of the influence that weak Rashba spin-orbit coupling has on the Kondo effect induced by a magnetic impurity in a two dimensional electronic system. It is shown that the Kondo effect is robust against such coupling of momentum and spin, despite the fact that the spin of the conduction electrons is no longer a conserved quantity. A proposal is made for how the spin-orbit coupling may change the value of the Kondo temperature \( T_K \) in such systems. Applications to semiconductor quantum dots and magnetic atoms on metallic surfaces are discussed.

12:15PM Y28.00006 Fano-Kondo effect in a two-level system with triple quantum dots, TETSUFI TANAMOTO, YOSHIFUMI NISHI, SHINOBU FUJITA, Advanced LSI Technology Laboratory, Toshiba Corporation — Quantum dot (QD) systems have been providing opportunities to probe a wide variety of many-body effects in microelectronic structures. Recently, the Fano effect, which appears as a result of quantum interference between a discrete single energy level and a major electronic system, has attracted the interests of many researches [1]. Here, we theoretically study the Fano-Kondo effect and Fano effect in a triple QD system, where two QDs constitute a two-level system and the other QD works in a detector with electrodes. When two QDs are coupled, bonding and anti-bonding states are formed. It is expected that the detector current reflects these electronic states. Indeed, we found that the Fano dip is modulated by strongly coupled QDs with a slow detector. We also compare noise properties of Fano-Kondo effect with those of Fano effect, and we found that, depending on the coupling strength among the QDs, noise and the Fano factor are greatly modulated for a slow detector. These suggest a new method of reading out qubit states [2]. 

12:27PM Y28.00007 Kondo physics with ac driving in the single electron transistor subjected to finite bias, ALI GOKER, Universite de Montreal — We employ the time-dependent non-crossing approximation to study the time averaged conductance for a single electron transistor in the Kondo regime when the dot level is sinusoidally driven from its equilibrium position by means of a gate voltage in finite bias. We find that the average conductance exhibits considerable deviation from the monotonous reduction when the applied bias is equal to the driving frequency of the dot level. We attribute this behaviour to the overlap of the satellite Kondo peaks with the split Kondo resonances formed at each lead’s Fermi level. We display the spectral function to put our interpretation into more rigorous footing. We also investigate the effect of the temperature and the driving frequency on the observed enhancement.

12:39PM Y28.00008 Interplay of Interactions and Phase Coherence in Open Quantum Dots, ILEANA RAU, MICHAEL GROBIS, RON POTOK, Stanford University, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDHABER-GORDON, Stanford University — The effect of Coulomb interactions on the electronic properties of a confined quantum system greatly weakens when electrons are allowed to rapidly enter and exit the system. For electron transport through a quantum dot, increasing the coupling of the dot to nearby leads causes a transition from the Coulomb blockade regime to a regime dominated by interference phenomena. We have investigated this transition in large, micron-sized quantum dots and found that Coulomb blockade effects persist in a regime where they had generally been assumed absent: when a dot is coupled by one fully transmitting mode to each of two leads. We discuss the interplay of these residual Coulomb interactions with phase coherent transport through a dot. We also examine how the subtle suppression of conductance by these Coulomb interactions affects the electron dephasing rate at low temperatures in open quantum dots.

12:51PM Y28.00009 Numerical estimate of correlation energy for two electrons confined in 2D quantum dot, TAKUMA OKUNISHI, YUKI NEGISHI, MASAKAZU MURAGUCHI, KYOZABURO TAKEDA, Waseda University — Local density approximation (LDA) is now widely accepted to design the novel materials as well as to predict new phenomena. In practical use of LDA, estimate of correlation energy is crucial. Tanatar et al. have given the well-known comprehensive expression of LDA correlation energy for 2D electron gas [1]. However, a straightforward use of this correlation energy for two electrons confined in 2D quantum dot is not possible. We have obtained the correlation energy for two electrons confined in 2D QD by applying the improved LDA. [1] B. Tanatar and D. M. Ceperley, Phys. Rev. B 39, 5005 (1989).
to acknowledge support from DOE Award Nos. DE-FG02-07ER46376 and DE-FG02-07ER46377. I.K. Hsu contact resistances can also be differentiated via the offset of the temperature increase at the ends of the suspended CNT. The results show the ratio of the

Fourier heat transport equation, we determine the thermal contact resistance ($R C T$) and correlate the CTE with the tube atomic structure. All the 4 walls of this individual MWCNT show apparent radial diameter thermal contraction. Because of the small size, experimental measurement of individual CNTs is very difficult; So far only limited data was reported by X-ray (CNTs). The coefficient of thermal expansion (CTE) of CNTs has been a subject of considerable debate in the literature with more recent works predicting, J. ZHANG, L. JI, J. ZUO, Univ. of Illinois — It is of fundamental value to understand the thermo-mechanical properties of individual carbon nanotubes (CNTs). The coefficient of thermal expansion (CTE) of CNTs has been a subject of considerable debate in the literature with more recent works predicting such anisotropic Casimir interaction has not been considered before and may lead to an orientation of long flexible objects, like nanotubes, at polar substrates. The interaction energy is derived analytically for the case of a single-wall nanotube on the ST-cut quartz. Besides a material dependent energy constant, it is proportional to the ratio of the volume of interacting segment of the nanotube and cube of the distance to the substrate. The interaction energy is derived analytically for the case of a single-wall nanotube on the ST-cut quartz. Besides a material dependent energy constant, it is proportional to the ratio of the volume of interacting segment of the nanotube and cube of the distance to the substrate.

This work was supported by U.S. DoE Grant DEFG02-01ER45923. Microscopy was carried out at the CMM at the MRL, which is partially supported by the U.S. DoE under grant DEFG02-91-ER45439.

**11:15PM Y28.00011 Non-Markovian Dynamics of Charge Carriers in Quantum Dots at High Bias** EDUARDO VAZ, JORDAN KYRIAKIDIS, Dalhouse University — We have investigated the dynamics of bound particles in multi-level current-carrying quantum dots. We look specifically in the regime of resonant tunneling transport, where several channels are available for transport: Through the non-Markovian Born-Redfield formalism, we investigate the real-time evolution of the confined particles including transport-induced decoherence and relaxation. In the case of a coherent superposition between states with different particle number, we find that coherence may be preserved even in the presence of tunneling into and out of the dot. Real-time results are presented for various asymmetries of tunnel barriers and tunneling rates into different orbitals.

Friday, March 14, 2008 11:15AM - 2:15PM –

Session Y29 DMP: Focus Session: Carbon Nanotubes and Related Materials XVI: Mechanical and Thermal Properties Morial Convention Center 221

**11:15AM Y29.00001 Anisotropic Casimir interactions between a one-dimensional object (nanotube) and a polar substrate**, SLAVA V. ROTKIN, Physics Dept, Lehigh University, ALEXEY G. PETROV, Liffe Institute, JOHN A. ROGERS, Beckman Institute, UIUC — The energy of Casimir interaction of a polarizable one-dimensional object (1DO), e.g. a nanotube, and a polar substrate was estimated. Within our model the energy of the dipole moment induced in the 1DO by the external electric field of the fluctuations of the quantized surface optical phonon modes is evaluated. Such polaron modes are known to exist in polar insulators and have the electric field with an exponentially decreasing wing in vacuum. If the polarization tensor of the 1DO is not isotropic, an orientation dependent Casimir force may arise. To the best of our knowledge, such anisotropic Casimir interaction has not been considered before and may lead to an orientation of long flexible objects, like nanotubes, at polar substrates. The interaction energy is derived analytically for the case of a single-wall nanotube on the ST-cut quartz. Besides a material dependent energy constant, it is proportional to the ratio of the volume of interacting segment of the nanotube and cube of the distance to the substrate.

**12:27AM Y29.00002 Dynamics and energy dissipation of nano-graphite mechanical devices**, ZHIPING XU, Rice University — Controllable mechanical motion of nano-structures holds great interest because of their applications in the nano-electromechanical systems (NEMS). One of the novel models proposed was the nano-graphitic materials based devices, where planar or cylindrical graphene layers act as moving parts and the motion is managed by the van der Waals force between them. Comparing with the multi-walled carbon nanotubes, nano-graphite flakes have an accessible scale for current techniques. Recent experiments using nano-mechanical manipulator have shown self-retraction motion of micrometer graphite layers after mechanical extrusion (Zheng et al. submitted to PRL). However, persistent oscillation as expected was not observed. The short lifetime implies severe energy dissipation. Analysis based on MD simulation show that the coupling with rotation and lattice vibration contribute significantly. Furthermore we have discussed the effects of edge instabilities, surface contamination and non-planar deformation, which also introduce complexities into the dynamics as approved by the experimental observation.

**11:39AM Y29.00003 Large Negative Thermal Expansion of an Individual Carbon Nanotube**

J. ZHANG, L. JI, J. ZUO, Univ. of Illinois — It is of fundamental value to understand the thermo-mechanical properties of individual carbon nanotubes (CNTs). The coefficient of thermal expansion (CTE) of CNTs has been a subject of considerable debate in the literature with more recent works predicting thermal contraction. Because of the small size, experimental measurement of individual CNTs is very difficult; So far only limited data was reported by X-ray diffraction that measured the average CTE of many tubes. Here, we use nanoarea electron diffraction to measure the CTE of an individual Multi-walled carbon nanotube (MWCNT) and correlate the CTE with the tube atomic structure. All the 4 walls of this individual MWCNT show apparent radial diameter thermal contraction. Because of the small size, experimental measurement of individual CNTs is very difficult; So far only limited data was reported by X-ray diffraction that measured the average CTE of many tubes. Here, we use nanoarea electron diffraction to measure the CTE of an individual Multi-walled carbon nanotube (MWCNT) and correlate the CTE with the tube atomic structure. All the 4 walls of this individual MWCNT show apparent radial diameter thermal contraction from 297 to 827 K, and thermal expansion from 827 to 1027 K. The radial CTE has strong direction dependence between 297 and 827 K. It changes from (-6.48±0.46) E-5 (1/K) for the wall with the theoretical diameter 16.4 Å to (-2.37±0.77) E-5 (1/K) for the wall with the theoretical diameter 37.3 Å, which means smaller diameter wall contracts more. On the other hand, all 4 walls of this individual MWCNT show apparent axial thermal contraction from 297 to 1073 K. The axial CTE is independent of the diameter, and the average axial CTE for different walls is (-1.30±0.07) E-5 (1/K).

This work was supported by U.S. DoE Grant DEFG02-01ER45923. Microscopy was carried out at the CMM at the MRL, which is partially supported by the U.S. DoE under grant DEFG02-91-ER45439.

**11:51AM Y29.00004 Optical Measurement of Thermal Contact Resistance in Suspended Carbon Nanotubes** I-KAI HSU, RAJAY KUMAR, ADAM BUSHMAKER, MICHAEL T. PETTES, LI SHI, TODD BRINTLINGER, MICHAEL S. FUHRER, JOHN CUMINGS, STEPHEN B. CRONIN, University of Southern California — We observe the local temperature increase profile $\Delta T(x)$ along suspended carbon nanotubes (CNTs) by converting the shifts in the $G$-band Raman mode to temperature. By deconvolving the temperature profile using the Fourier heat transport equation, we determine the thermal contact resistance ($R C T$) relative to the intrinsic thermal resistance of the nanotube itself ($R_N T$). The curvature of the temperature profile is found to be dominated by the ratio of $R_N T$ to $R C T$. The contact resistance can also be differentiated via the offset of the temperature increase at the ends of the suspended CNT. The results show the ratio of the contact thermal resistance to the nanotube thermal resistance to range from 0.02 to 17. The measurement is also able to distinguish between ballistic and diffusive thermal transport. We find diffusive thermal transport to dominate the heat transport in all nanotubes measured in this study. The authors would like to acknowledge support from DOE Award Nos. DE-FG02-07ER46376 and DE-FG02-07ER46377. I.K. Hsu et al., Applied Physics Letters (in press).
12:03PM Y29.00005 Thermal Conductance Measurement of Metal-CNT Composites using Micro-Sized Suspended Structure, KI SUNG SUH, JUNG HOON BAK, BYUNG YANG LEE, SEUNGHUN HONG, YUN DANIEL PARK, FPRD Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — As CNTs have a unique structure and remarkable physical properties, CNT composites have attracted much attention from many researchers. Especially the thermal properties of CNTs and their composite materials have been studied intensively, because CNT has very good thermal transport properties [1-5]. For example, thermal conductivity of CNT is known to be much larger than that of metals such as Ag, Au, Cu and Al. To study the thermal conductance of metal-CNT composites, we have fabricated the micro-sized suspended structures. By using e-beam lithography and metalization, two thermometers have been patterned on the GaAs substrates. Thermal links made of metal or metal-CNT composite also have been patterned between the two thermometers. Then GaAs substrate has been under-etched to form suspended structures. We will show the fabrication methods and measurement scheme using these microstructures. * parkyd@phy.snu.ac.kr [1] J.A. Eastman et al., Appl. Phys. Lett. 78, 718 (2001). [2] S.U.S. Choi et al., Appl. Phys. Lett. 79, 2252 (2001). [3] M.J. Biercuk et al., Appl. Phys. Lett. 80, 2767 (2002). [4] R. Ramasubramaniam et al., Appl. Phys. Lett. 80, 4647 (2003). [5] H.Q. Xia et al., Appl. Phys. Lett. 94, 4967 (2003).

12:15PM Y29.00006 Thermal conductivity of isolated and interacting carbon nanotubes, DAVIDE DONADIO, GIULIA GALLI, UC Davis — We have investigated the thermal conductivity of single wall carbon nanotubes (SWCNT) either isolated or in contact with external media, by using equilibrium molecular dynamics and the Boltzmann transport equation. We show that, contrary to existing controversies, both methods yield a finite value of the thermal conductivity for infinitely long tubes, as opposed to the case of 1D momentum conserving systems. Acoustic and flexure modes with mean free paths of the order of a few micron, as observed also in experiments, are identified as major contributors to the high value of SWCNT conductivity. We also find that the interaction with an external medium may substantially decrease the lifetime of the low frequency vibrations, reducing the thermal conductivity by up to two orders of magnitude.

12:27PM Y29.00007 Determination of carbon nanotube wall thickness and elasticity by atomic force microscopy, TRISTAN DEBORDE, CALEB JOINER, MATTHEW LEYDEN, ETHAN MINOT, Oregon State University — To understand the operation of carbon nanotube (CNT) devices it is important to determine whether nanotubes are single-walled or multi-walled. Transmission electron microscopy of CNTs has previously been the only tool available to count the number of graphene sheets forming the wall of a CNT. We show that atomic force microscopy can measure CNT wall thickness by squeezing individual nanotubes between a tip and a hard surface. Full compression of single-walled and double-walled CNTs can be achieved either by a static force or by ac-mode imaging, allowing clear determination of wall number. Direct measurements of compression forces are used to determine the elastic properties of the wall, yielding the bending modulus of graphene.

12:39PM Y29.00008 Pressure Induced Changes in the Atomic and Electronic Structure of Carbon Nanotubes, SUMIT SAXENA, TREVOR A. TYSON, New Jersey Institute of Technology - Newark — We present first principle density functional calculations on small diameter single walled carbon nanotubes to explore the changes in their electronic structure and atomic arrangement under hydrostatic compression. Simulations on zigzag (n, 0) SWCNT 6 ≤ n ≤ 9 using the full potential projector augmented wave and ultra-soft pseudo potentials were conducted. Large structure-related changes are found in the density of states at the Fermi energy. The cross sections of small tubes exhibits deformations not predicted by classical models. The structural cross sections of large diameter tubes calculated under moderate pressure are consistent with the reported results. The details of calculations and other results will be presented. This work is supported in part by NSF DMR-0512196.


12:51PM Y29.00009 Nanomechanical energy transfer in carbon nanotubes: fundamental insights from molecular dynamics simulations, GIOVANNA LANI, Politecnico di Torino, Torino, Italy and Center for Integrated Nanomechanical Systems (COINS), University of California, Berkeley., P. ALEX GREANEY, COINS, University of California, Berkeley, GIULIA GALLI, UC Davis, TRISTAN DEBORDE, CALEB JOINER, MATTHEW LEYDEN, ETHAN MINOT, Oregon State University — To understand the operation of carbon nanotube (CNT) devices it is important to determine whether nanotubes are single-walled or multi-walled. Transmission electron microscopy of CNTs has previously been the only tool available to count the number of graphene sheets forming the wall of a CNT. We show that atomic force microscopy can measure CNT wall thickness by squeezing individual nanotubes between a tip and a hard surface. Full compression of single-walled and double-walled CNTs can be achieved either by a static force or by ac-mode imaging, allowing clear determination of wall number. Direct measurements of compression forces are used to determine the elastic properties of the wall, yielding the bending modulus of graphene.

1.03PM Y29.00010 A Failure Criterion for Single-Walled Carbon Nanotubes Based on Molecular Mechanics, ANTONIO AVILA1, Univesidade Federal de Minas Gerais, GUILHERME LACERDA, Universidade Federal de Minas Gerais — Single-walled carbon nanotubes (SWNT) are the natural choice for high performance materials. The problem, however, arises when the experimental data are compared against each other. The large variability of experimental data lead to development of a new set of numerical simulations called molecular mechanics, which is a “symbiotic” association of molecular dynamics and solid mechanics. This paper deals with a molecular mechanics simulations of single-walled carbon nanotubes. Three SWNT configurations and their combinations were simulated, i.e. armchair, zigzag and chiral. The failure criterion introduced is based on modified Morse’s potential with dissociation energy of 124 Kcal/mol and an inflection point considered is around 13% of strain. The numerical data are in agreement with data from Belytschko et al. (2002) where the failure occurred at 10.6% strain at 65.2 GPa of stress. To be able to identify the highest stress concentration region, one end of the SWNT all degrees-of-freedom were fixed and a prescribed axial displacement was applied at the opposite end. The Sadoc (chiral-chiral) configuration had the highest stress at the smallest chiral SWNT. For the Dunlap configuration (chiral-zigzag) the highest stress occurred at chiral part close to the pentagon location.

1. Associate Professor
1:15PM Y29.00011 Excitons in Single-Walled Carbon Nanotubes in Different Local Environments: Effects of Strain and Disorder on Magnetic Brightening

T. A. SEARLES, ECE Dept, Rice University, D.J. HILTON, J. SHAPER, W.D. RICE, Rice Univ, Y.-D. JOH, GIST, Korea, S.A. MCGILL, NHMFL, J.A. FAGAN, E.K. HOBIE, NIST, J. KONO, ECE Dept, Rice University — Recent experiments on single-walled carbon nanotubes (SWNTs) have shown that in the presence of a high magnetic field the two lowest-energy spin-singlet exciton states become bright [1]. Furthermore, this “magnetic brightening”, or increase in photoluminescence (PL) intensity as a function of magnetic flux through each SWNT, increases as the temperature decreases. Here, we report results of temperature-dependent magneto-PL from 2 to 200 K and up to 45 T on SWNTs of the same stock solution suspended in four different local environments. We compared both the brightening and temperature dependence of tubes stretch aligned and unaligned in poly-acrylic acid matrices. As expected, the tubes aligned at high magnetic field exhibited more brightening than those unaligned. We also investigated the behavior of SWNTs in two other matrices, iota-Carrageenan and gelatin. Along with the expected peak shifting and broadening from the effects of strain, we found that the temperature dependence changes with local environment. [1] S. Zaric et al., PRL 96, 016406 (2006); J. Shaver et al., Nano Lett. 7, 1851 (2007); I. B. Mortimer and R. J. Nicholas, PRL 98, 027404 (2007).

1We would like to acknowledge support from the Welch Foundation, NSF No. DMR-0084173, the State of Florida, and DOE. T. A. Searles would like to thank the ONR/HBEC FEFF Fellowship Program.

1:27PM Y29.00012 Carbon nanotube nanomechanical mass sensors

HSIN-YING CHIU, PETER HUNG, California Institute of Technology, HENK POSTMA, California State University Northridge, MARC BOCKRATH, California Institute of Technology — Single-walled carbon nanotubes are arguably the lightest and smallest wires in the world, and have recently been shown to act as nanomechanical resonators [1]. As a result, single-wall carbon nanotubes are excellent candidates for highly sensitive mass sensing [2]. We observed the down shift of the resonant frequency of a suspended double-clamped carbon nanotube resonator at cryogenic temperatures upon helium mass loading. Using a straightforward estimate of the nanotube mass, the observed frequency shift corresponds to the mass of ~1000 helium atoms, which is the zeptogram range. This is considerably smaller than found previously with nanotube resonators, and comparable to that found using nanowire resonators [3]. Our noise floor is currently ~1 Xenon atom per root Hz, which may enable single-atom detection in future experiments. [1] Vera Sazonova, et al., Nature 431, 284 (2004). [2] H. B. Peng, et al. Phys. Rev. Lett. 97, 087203 (2006) [3] Y. T. Yang, et al. Nano Lett. 6, 583 (2006).

1:39PM Y29.00013 Anharmonic phonon lifetimes in carbon nanotubes, graphene and graphite

NICOLA BONINI, Department of Materials Science and Engineering, MIT, Cambrige, MA, USA, MICHELE LAZZERI, FRANCESCO MAURI, Institut de Minologie et Physique des Milieux Condenses, Paris, France, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA — In this work we present a first-principles study of the anharmonic phonon lifetimes of the key vibrational modes that most strongly interact with electrons in carbon nanotubes, graphene and graphite. The calculations of both harmonic and anharmonic properties are performed using density-functional theory and density-functional perturbation theory. Our results—in excellent agreement with the available experimental data—provide a microscopic characterization of the energy relaxation mechanisms and of the relative importance of the individual decay channels. We will discuss the relevance of these results to elucidate the role of non-equilibrium phonon populations in high-field electronic transport.

1:51PM Y29.00014 Measurement of mechanical properties of graphene using nanoindentation

CHANGGU LEE, XIADONG WEI, JEFFREY KYSAR, JAMES HONE, Columbia University — Mechanical properties of graphene have been measured using AFM nanoindentation. Mono-, bi-, and tri-layer graphene sheets are suspended over micron-sized circular hole arrays. Force-displacement curves obtained by AFM nanoindentation allow the extraction of mechanical properties such as Young’s modulus and fracture strength using equations for thin circular membranes. In order to verify the validity of the equations, the experimental and analytical results were compared with finite element simulation. The analytical equations fitted to the measurements show that Young’s modulus is 0.9-1.2 TPa and the fracture strength is 90-150 GPa for up to 3 layers.

2:03PM Y29.00015 Electrical conductivity of individual, thermally reduced graphene oxide sheets

INHWA JUNG, DMITRIY DIKIN, Northwestern University, Evanston, Illinois, RICHARD PINER, ROD RUOFF, University of Texas at Austin — Electrical properties of individual graphene oxide sheets were investigated. Graphene oxide itself is insulating, but its conductivity is finite and measureable following heat treatment in vacuum. The dependence on temperature and time for reduction of graphene oxide were fit to a standard chemical kinetics rate law and from this an activation energy of 30 kcal/mole was found. I-V curves, obtained at several stages of the chemical reduction achieved by heating, are non-linear and slightly asymmetric. The effect of applying an electric field via a back gate and the resulting change in resistance was measured at different temperatures and at different stages of reduction. The maximum conductivity by thermal annealing graphene oxide sheets was 85 S/m at room temperature and zero gate potential. This value was determined based on 4-probe pseudo Van der Pauw measurements and numerical modeling and using 1.0 nm as the sheet thickness.

1Supported by the NASA through the University Research, Engineering, and Technology Institute on Bio-inspired Materials (BiMat) and by the DARPA Center on Nanoscale Science and Technology for Integrated Micro/Nano-Electromechanical Transducers (iMINT).

Friday, March 14, 2008 11:15AM - 2:15PM — Session Y30 DCMP: Low Dimensional Systems Morial Convention Center 222

11:15AM Y30.00001 Inelastic neutron scattering from confined molecular oxygen

PAUL SOKOL, DUNCAN KILBURN, Indiana University — We report results from experiments measuring the generalized density of states in confined solid molecular oxygen. It is known from previous experiments that fundamental properties of liquids and solids, such as phase transition temperatures and intermolecular structure can be altered by confining them in porous media (pores typically in the angstrom to nanometer range). It is reasonable therefore to ask the question: what is the effect of confinement on collective excitations in the material, and can these changes be exploited in a technological setting? Using inelastic neutron scattering we find that both the structure and generalized density of states of solid molecular oxygen are altered by confining it in a templated porous glass with a mean pore diameter of 100 Angstroms. The structure, in the Q-range which we were able to measure, resembles that of an amorphous material and the density of states is shifted to lower energy excitations. One possible application for such a material is as moderator material in a very cold neutron source.

1This work is supported by the National Science Foundation.
11:27AM Y30.00002 Imaging One-Electron Quantum Dots in InAs/InP Nanowires

HALVAR TRODAHL, ERIN BOYD, R.M. WESTERVELT, Harvard University, LINUS FROBERG, LARS SAMUELSON, Lund University — Quantum dots formed in InAs/InP heterostructure nanowires are attractive candidates for nanoelectronics, spintronics, and quantum information processing. It has been shown that with the use of a liquid helium cooled scanning probe microscope (SPM) the electronic charge state of a single quantum dot can be chosen by merely moving the tip of the SPM with respect to the dot [1]. Simulations show that this technique can also be implemented for double quantum dots with interdot separation less than 30nm. By applying a magnetic field the electronic states of a quantum dot can be split. It is possible to image this splitting with the local, movable electrostatic gating of the SPM. A magnetic field applied to a double dot system can be used to create a spin filter; a simple movement of the SPM tip with respect to the dot structure can determine which spin passes through the filter.


11:39AM Y30.00003 Imaging the Wavefunction of a One-Electron Quantum Dot

ERIN E. BOYD, HALVAR J. TRODAHL, Dept of Physics, Harvard Univ, PARISA FALLahi, Dept of Physics, ETH, R.M. WESTERVELT, Dept of Physics and Sch of Eng and App Sci, Harvard Univ, LINUS E. FROBERG, LARS SAMUELSON, Dept of Solid State Physics, Lund Univ — InAs quantum dots grown in InAs/InP nanowires are promising contenders for nanoelectronics. A fundamental understanding of the quantum behavior of the electron is important for the design of quantum devices. We have developed an imaging technique to image the electron wavefunction of a quantum state inside a long InAs dot (length>diameter) formed by InP barriers, using a liquid He-4 cooled scanning probe microscope [1]. The electrostatic potential of the tip dents the wavefunction and changes the energy of the quantum state by an amount proportional to the electron probability density at the tip position. Using Coulomb blockade conductance images of the dot, the energy change vis. tip position can be found. By deconvolving the measured energy shift with the tip potential, one can extract the electron probability density, using first-order perturbation theory. [1] P. Fallahi, PhD Thesis, Harvard Univ (2006).

11:51AM Y30.00004 Theoretical study of spin relaxation in a carbon nanotube quantum dot

BRIAN BEZANSON, XUEDONG HU, SUNY Buffalo — Carbon nanotubes offer an attractive environment for coherent spin manipulation due to the small population of nuclear spins and weak spin-orbit interaction. While a couple of specific spin relaxation mechanisms have been investigated theoretically[1][2], there is still no comprehensive study of spin lifetimes in carbon nanotubes. In the present study we calculate the spin decay rate for electrons in gate-defined quantum dots on carbon nanotubes due to the spin-orbit and electron-phonon interactions. More specifically, we explore effects of magnetic field strength and orientation, tube diameter and chirality, and confinement.


12:03PM Y30.00005 Analysis of unusual splitting of Kondo peak in the differential conductance of a carbon nanotube quantum dot

JEFFREY STEPHENS, JEROME LICINI, Lehigh University, A.T. CHARLIE JOHNSON, DOUG STRACHAN, DANVERS JOHNSTON, SAM KHAMIS, University of Pennsylvania — Carbon nanotubes grown by chemical vapor deposition on an oxidized silicon substrate were contacted to form a gated sample of parallel tubes. Testing was done at low temperature and high magnetic field using a dilution refrigerator and superconducting magnet. The current versus voltage graph shows asymmetry with respect to zero volts. The differential conductance (dI/dV) is computed and yields some intriguing behavior. The previous asymmetry is more apparent as is a sharp increase in conductivity near zero volts. Temperature data further suggests a conductance peak at near zero voltage consistent with the Kondo effect. High magnetic fields, 0 to 11 Tesla in 0.5 Tesla increments, are used to probe the conductance behavior. The magnetic field tests yield unusual shapes and splitting at two critical fields.

12:15PM Y30.00006 Probing edge-localized states of graphene quantum dots on Co(0001)

DAEJIN EOM, KWANG RIM, DUII ZHOU, MICHAEL LEFENFELD, LI LIU, SHENXIONG XIAO, COLIN NUCKOLLS, GEORGE FLYNN, TONY HEINZ, Columbia University — Two-dimensional graphene sheets of finite lateral extent are expected to show characteristic edge states at their boundaries. In particular, for zigzag edges, highly degenerate localized states have been predicted theoretically (Ref. 1) and probed by STM (Ref. 2). Such boundary effects are expected to be particularly prominent for nanometer-scale graphene quantum dots, structures for which the proportion of edge atoms is significant. In this paper we present investigations of graphene quantum dots that we have prepared by annealing carbon- bearing precursor molecules on a Co(0001) surface. Using scanning tunneling microscopy as a local probe of the physical and electronic structure, we report results on the nature of edge states for quantum dots of differing geometrical shape. We observed prominent edge-localized states for triangular quantum dots, whereas these features are suppressed for quantum dots of hexagonal shape. These observations are consistent with numerical simulations of the expected electronic structure. 1. M. Fujita et. al., J. Phys. Soc. Jpn. 65, 1920 (1996) 2. Y. Niimi et. al., Phys. Rev. B 73, 085421 (2006)

12:27PM Y30.00007 Surface Functionalized Carbogenic Quantum Dots

A. B. BOURLINOS, NCSR “Demokritos”, Greece, A. STASSINOPoulos, A. ANGLOS, S.H. ANASTASIADIS, Foundation for Research and Technology-Hellas, Greece, R. ZBORIL, Palacky Univ., Czech Republic, M. KARAKASSIDES, Univ. of Ioannina, Greece, E.P. GIANnELIS, Cornell Univ — Surface functionalized carbon-based quantum dots (C-QDs) are formed in-situ in a single-step process via thermal carbonization of suitable molecular precursors based on ammonium citrate salts. The as-synthesized nanoparticles have near spherical morphology and size around 7nm. Using different surface modifiers, we can form hydrophobic or hydrophilic capped C-QDs, which can be dispersed in organic or aqueous solvents, respectively. These C-QDs fluoresce strongly upon optical excitation. We believe that the fine size of the C-QDs combined with their disorder structure favor a high concentration of defect sites at the surface of the nanoparticles that, upon stabilization by the attached organic groups, give rise to the observed emissions. It is further noted that the emission band shifts to shorter wavelengths as the excitation is blue-shifted. In a series of studies, the emission quantum yield of C-QDs was found to be around 4%. These types of materials are promising as fluorescent tags for biological application. Sponsored by the UlfFORTH (Laserlab- Europe) and by the Greek GSRT.

1 Also at Aristotle Univ. of Thessaloniki, Greece
12:39PM Y30.00008 Scanning Probe Microscopy Characterization of Electrical Properties of Bimetallic Core Shell Nanostructures, REGINA RAGAN, SANGYEOB LEE, ANIKAETA SHINDE, SATORU EMORI, UC Irvine — Metallic nanoparticles have shown enhanced catalytic activity compared to their bulk counterparts potentially due to changes in electronic properties at the nanoscale. Challenges in nanoscale catalysis studies include the fabrication of monodisperse nanostructures as well as a fundamental knowledge of the electronic properties at the nanometer length scale. Our group addresses these issues by fabricating dense ordered arrays of bimetallic core-shell nanostructures and characterizing structures with scanning tunneling spectroscopy and Kelvin probe force microscopy. Self assembled rare earth disilicide nanowires are used as templates for the growth of the structure. We will present results on the electronic and vibrational properties of these structures with nanometer scale resolution using STS and KPFM. STS measurements of RESi2 nanowires will be presented that show enhanced tunneling as compared to thin films as well as size dependant rectification ratios when comparing islands and wires of various width. KPFM is used to measure the work function of various sizes of RESi2 nanostructures providing a fundamental basis for understanding catalytic behavior in terms chemical activity of the nanostructures. KPFM data reveals a higher CPD for DySi2 nanowires than islands with Δφ nanoisland-nanowire found to be 230mEV.

12:51PM Y30.00009 Controlled fabrication and electrical properties of long quasi-one-dimensional superconducting nanowire arrays, KE XU, JAMES HEATH, Division of Chemistry and Chemical Engineering, California Institute of Technology — Quasi-one-dimensional superconducting nanowires are an interesting and ideal system to examine fundamental superconducting phase transition phenomena. We report a general method for reliably fabricating quasi-one-dimensional superconducting nanowire arrays, with good control over nanowire cross section and length, and with full compatibility with device processing methods. We investigate Nb nanowires with individual nanowire cross-sectional areas that range from bulk-like to 10 x 11 nm, and with lengths from 1 to 100 micrometers. Nanowire size effects are systematically studied. In particular, a comprehensive investigation of influence of nanowire length on superconductivity is reported for the first time. All results are interpreted within the context of phase-slip models.

1 This work was supported primarily by the Department of Energy (DE-FG02-04ER46175), with additional support from the Office of Naval research (N00014-07-1-0360) and the MARCO Center for Advanced Materials and Devices.

1:03PM Y30.00010 Optical Interferometry of Gas Pressure Damped Silicon Nanobridges and Nanocantilevers, O. SVITELSKY, N. LIU, V. SAUER, J. LOSBY, M. BELOV, E. FINLEY, K.M. CHENG, M. FREEMAN, W. HIEBERT, University of Alberta Physics Dept, and National Institute for Nanotechnology, Edmonton AB Canada — The growing interest in NEMS, in particular in nanobridges and nanocantilevers, is determined by the prospective of their use as highly sensitive sensors of various physical factors: mass, tension, pressure, viscosity, etc. In order to investigate their properties under damping, a series of NEMS with different sizes was prepared from standard SOI wafers by the chemical etching after electron beam lithography. The surfaces were coated by layers of Al, Au and/or Cr in different combinations. The quality of the fabricated NEMS was evaluated by SEM imaging. The resonant frequencies of the NEMS varied in the range of 10-1000 MHz. The damping was introduced by means of pressurized gas in specially built optical pressure chamber capable to hold up to 5 atmospheres with glass window and not less than 160 atmospheres if equipped with sapphire window. We demonstrate that the NEMS Q-factor, the amplitude and the frequency of their resonances show considerable dependence on the value of the pressure in the chamber.

1:15PM Y30.00110 Periodic and Quasiperiodic Nanostructures: Accessing Complex Architectures Through Designer Phase Masks, CHEONG YANG KOH, EDWIN THOMAS, Massachusetts Institute of Technology — In this work, we show how one may design phase mask architectures in order to achieve complex 3-dimensional periodic and quasiperiodic nanostructures through considerations of the symmetries of the phase masks. By making use of the fact that phase mask interference lithography is essentially a case of light propagation through the non-modulated direction of a finite photonic crystal slab, we show that the diffracted beams obey the symmetry restrictions of the corresponding phase mask, which allow us to determine and design the polarizations and directions of the exiting beams which interfere coherently in the substrate, subsequently leading to the formation of 3-dimensional nanostructures which are periodic or quasiperiodic. The extension of this approach towards quasiperiodic structures is straightforward when working in Fourier space, which identifies the propagating eigen-modes within the phase mask, or photonic crystal slab. This allows us to rationally design structures with targeted properties, utilizing this Fourier space approach. We show several examples of this approach in achieving this method of fabrication for both periodic and quasiperiodic nanostructures.

1 NSF, ISN

1:27PM Y30.00112 Field Emission Enhancement and the Field-Screening Effect Reduction using Carbon Nanopipettes as Cold Cathodes, ABDELILAH SAFIR, ElectroOptics Resarch Institute and Nanotechnology Center, University of Texas at Austin, THE CENTER FOR COMPLEX QUANTUM SYSTEMS TEAM — We compute the electron transmission through a bi-ripple waveguide. The dimensions of the bi-ripple waveguide is A) demonstrates promising emission properties of graphene.

1:39PM Y30.00013 Dicke effect in a multi-ripple electron waveguide, HOSHIK LEE, LINDA REICHL, The University of Texas at Austin, THE CENTER FOR COMPLEX QUANTUM SYSTEMS TEAM — We compute the electron transmission through a bi-ripple electron waveguide. We numerically observe a resonance splitting, in this open quantum system, which is analogous to the Dicke effect in quantum optics. We also plot S-matrix poles in the complex energy plane, and find that two symmetry related poles contribute to the resonance splitting. We find that the symmetric resonant states are easily coupled to the leads, but the anti-symmetric states are not. We show the resonance splitting is due to a indirect interaction between wavefunctions in each cavity using a simple model. We also show that one of S-matrix poles withdraws from the real axis as a ripple is added. It turns out that the width of the resonance for N-ripple waveguide is N times larger than the resonance width of a mono-ripple waveguide. It agrees with the result of the Dicke model.

1:51PM Y30.0014 What is Quantum in Quantum Pumping: The role of the Phase and Asymmetries, KUNAL NAS, Fordham University, TOMAS OPATRNY, Palacky University — By studying several examples, we show that quantum pumping does not always necessitate a strictly quantum description, neither is phase always a necessary concept. The same quantum mechanical picture of pumping encompass a variety of distinct mechanisms, some can be simulated by classical mechanisms while others can be explained only in a quantum picture; the role of the phase of the wavefunction is the crucial differentiator. We also show that most pumping processes have a previously unconsidered antisymmetric component which contributes significantly to the instantaneous current at each terminal but causes no net charge transfer. We have also computed the exact pumped current for arbitrary rates of time variation for certain potentials, not just in the adiabatic regime as has been previously studied.
2:03PM Y30.00015 Evanescent-wave current through nanometer-scale conductor with generalized channel decomposition in non-equilibrium Green’s function theory, HIROSHI SHIINOAKA, Dept. of Applied Physics, Univ. Tokyo, TAKEO HOSHI, Dept. of Applied Mathematics and Physics, Tottori Univ. and JST-CREST, TAKEO FUJIIWARA, Center for Reserch and Development of Higher Education, Univ. Tokyo and JST-CREST — In optics, evanescent wave is known as a decay mode without dissipation, which appears at total reflecting surfaces and surfaces of nanoparticles. Even though such decay mode can be found, in principle, also in electronic current in nanometer-scale conductors, the evanescent wave effect has not yet been investigated systematically, in materials with electronic structure. We present a new eigen-channel decomposition of Green’s function and the associated effective medium approximation. By applying this method and knowing the system is located at a nanometal wires, we found decaying behavior of electron density and backward current flows near electrodes, which is evidence of evanescent waves. We also found that the evanescent waves cause conductor-length dependence of the transmission, which is detectable in experiments. Dependence of the evanescent waves on materials and structures are also discussed from a point of view of band structures and their connectivity at electrodes.

This work was supported by JSPS Research Fellowships for Young Scientists.

Friday, March 14, 2008 11:15AM - 2:03PM – Session Y31 DMP GMAG: Focus Session: Sodium Cobaltites Morial Convention Center 223

11:15AM Y31.00001 Charge order and anomalous magnetism in the Na cobaltates, HENRI ALLOUL, Physique des Solides, CNRS UMR 8502, univ. Paris-Sud, 91405 ORSAY — The layered Na cobaltates have some analogies with the cuprates as 2D conductivity occurs in the CoO planes and doping can be modified by changing the Na content. Also ordered magnetic phases have been evidenced, but unexpectedly for large values of x for which one would expect a hole doping of the band insulator NaCoO₂. Indeed, in the high crystal field on the Co sites in these compounds, an anionic picture for the Co states would correspond to low spin configurations Co³⁺, S=0 or Co⁴⁺, S=1/2. We shall present SQUID and $^{23}$Na and $^{59}$Co NMR data [1] taken on samples synthesized and characterized by X ray crystallography in LLB, Saclay. We evidence that the Co charge is uniform for x=0.35 as in the hydrated superconductive phase. For high Na contents the samples are found to display ordered Na structures or mixtures of those, with different x values. In pure phases isolated for specific x values, we evidence a charge disproportionation into non magnetic Co⁵⁺ and more magnetic Co sites with an average charge of about Co⁴⁺, except for x=0.5 [2]. This hole delocalization and charge order occur both for paramagnetic and AF phases [3]. NMR investigations of the dynamic susceptibilities allow us to characterize the nature of the in plane electronic correlations in most parts of the phase diagram. Contrary to the case of most cuprates for which dopant disorder is quite influential, the hole doping achieved in cobaltate samples is associated with the insertion of well ordered Na planar structures. They have to be taken into account to explain theoretically the metallicity, the magnetic properties and their evolution with doping.


11:51AM Y31.00002 Sodium Ordering Phase Transition in Sodium Cobaltate, D.J.P. MORRIS, HMI Berlin, Germany, M. ROGER, CEA Saclay, France, D.A. TENNANT, HMI Berlin and Technische Universitat Berlin, Germany, M.J. GUTMANN, ISIS Facility, UK., J.P. GOFF, Royal Holloway, University of London, UK., D. PRABHAKARAN, Clarendon Laboratory, Oxford, UK., J.-U. HOFFMANN, R. FEYERHERM, E. DUDZIK, K. KIEFER, HMI Berlin, Germany. — NaₙCoO₂ has emerged as a system of fundamental scientific interest because of its highly unusual electrical and magnetic properties. Using neutron and x-ray diffraction we have detected long-range 3D ordering of Na⁺ ions in single crystals, and demonstrate a kaleidoscope of Na⁺ ion patterns as a function of concentration and temperature [1]. Large scale numerical simulations reveal the ordering principle for this system, the formation of tri-vacancy charged droplets that then order long range, and the structure factors from these defect clusters are in good agreement with the observed neutron diffraction intensities. Superstructure transitions are observed in the diffraction data which are explained by a change from a stripe structure of tri-vacancies. The results readply explain many of the observed electrical and magnetic properties, including the formation of ferromagnetic sheets in the CoO₂ layers over this composition range, and the 3D nature of the magnetic excitations. [1] M. Roger et al. Nature 445, 631 (2007)

12:03PM Y31.00003 New magnetic states in Na₅CoO₂ induced by controlled Na order, T. F. SCHULZE, P. S. HAEFLIGER, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland, CH. NIEDERMAYER, Laboratory for Neutron Scattering, ETH Zurich, CH-8093 Zurich, Switzerland and Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland, K. MATTENBERGER, S. BUBENHOFER, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland — We prove the direct link between low temperature magnetism and high temperature Na⁺ ordering in Na₅CoO₂ using the example of a so far unreported magnetic transition at 8K. The new magnetic state carries a weak ferromagnetic moment parallel to the CoO₂ layers. The 8K feature has been characterized in detail and its dependence on a diffusive Na⁺ rearrangement around 200K is demonstrated. The diffusive process is found to slow down around 200K, and the characteristic time scale reaches several hours at 195K. Applying muons as local probes this process is shown to result in a reversible phase separation into distinct magnetic phases that can be controlled by specific cooling protocols. Thus the impact of ordered Na⁺ Coulomb potential on the itinerant electrons in the CoO₂ layers is evident, and new ways to experimentally revisit the Na₅CoO₂ phase diagram are discussed.

12:15PM Y31.00004 Precise control of the Na nonstoichiometry in Na₅CoO₂, YOSHIIKO OKAMOTO, ATSUISHI NISHIO, YOKO KIUCHI, ZENJI HIROI, Institute for Solid State Physics, Univ. of Tokyo — Na₅CoO₂ has been attracting great interests in terms of a correlation between its electronic properties and Na nonstoichiometry. Many groups have reported that a Na rich phase (x ~ 0.7) is a Curie-Weiss metal and a poor phase (x ~ 0.3) is a Pauli paramagnetic metal. The origin of this difference, however, has not been confirmed yet, mainly because of difficulty in controlling precisely the Na nonstoichiometry. We succeeded in synthesizing a series of polycrystalline samples of Na₅CoO₂ with well-controlled Na content by the solid-state reaction instead of the solution reaction previously used. We prepared polycrystalline Na₅CoO₂ (0.58 < x < 0.63) by a solid-state reaction of Na₀.₆₂CoO₂ and Na₀.₅₃CoO₂ at 200°C. Furthermore, fine tuning of Na content in the range of 0.62 < x < 0.63 was carried out by a solid-state reaction of Na₀.₆₂CoO₂ and Na₀.₅₃CoO₂. Magnetic susceptibility of Na₅CoO₂ exhibited Curie-Weiss behavior at x > 0.62 while nearly temperature independent paramagnetic behavior at x < 0.61. Such a drastic change of magnetism clearly indicates that the magnetic phase boundary is located in an extremely narrow range around x = 0.62. We think that the difference originates from a change of the Fermi surface topology with electron filling probably associated with the dip in the a₁g band near the Γ point.

12:27PM Y31.00005 Systematic ARPES study on Na-rich Na₅CoO₂ (0.75<x<1) Y.-M. MU, Boston College, P. RICHARD, M. NEUPANE, F.-C. CHOU, C.-T. LIN, M. GAO, Z. WANG, H. DING — The phase diagram of the cobaltolate Na₅CoO₂ with varying Na concentration x is very rich and complicated. At the high-doping regime (x>0.75), the system was found to be more correlated, with a spin-density-wave state emerging at low temperatures. A stable phase was found with $\sqrt{13} \times \sqrt{13}$ symmetrical superstructure at Na-rich doping cobaltite. We will report our recent ARPES results of the Na-rich Na₅CoO₂ (0.75<x<1) samples.
12:39PM Y31.00006 Fermi surface pockets in Na$_x$CoO$_2$ for $x = 0.71$ and 0.84: Localization effects and emergence of a spin-liquid ground state. LUIS BALICAS, YOUNJUNG JO, National High Magnetic Field Lab, Florida State University, Tallahassee, FL 32310, FANGCHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan. PATRICK LEE, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — Here we report the observation of Fermi surface (FS) pockets via the Shubnikov de Haas effect in Na$_x$CoO$_2$ for $x = 0.71$ and 0.84, respectively. Our observations indicate that the FS of each compound can intersect their corresponding Brillouin zones, as defined by the previously reported superlattice structures, leading to small reconstructed FS pockets, only if a precise number of holes per unit cell is localized. For $0.71 < x < 0.75$ the coexistence of itinerant carriers and localized $S = 1/2$ spins on a paramagnetic triangular lattice leads, at low temperatures, to the observation of non Fermi-liquid behavior in the electrical transport and heat capacity properties. Namely, an anomalous exponent in the temperature dependence of the resistivity and a logarithmic divergence of the heat capacity divided by temperature as the temperature is lowered. These observations suggest the possibility of a unique quantum spin-liquid ground state resulting from the interplay between itinerant carriers and fluctuating $S = 1/2$ spins on a frustrated lattice.

12:51PM Y31.00007 ARPES investigation of the electronic properties of PdCoO$_2$\textsuperscript{1}, I.M. VISHIK, W.S. LEE, Stanford University, H. TAKATSU, Kyoto University, D.H. LU, R.G. MOORE, Stanford University, Y. MAENO, Kyoto University, Z.-X. SHEN, Stanford University — The triangular-lattice layered cobaltates have emerged as an exciting new correlated electron system. Although tremendous progress has been made with Sodium Cobaltate (Na$_2$CoO$_2$) there still remain disputes, most notably, the precise Fermi surface topology. In order to gain another perspective, we have studied a related compound, Palladium Cobaltate (PdCoO$_2$). This is a chemically stably metallic oxide that can be prepared with very high purity, allowing us to study a clean system that lacks the complications introduced by doping in Na$_2$CoO$_2$. We present the first ARPES measurements on PdCoO$_2$, focusing on determining the Fermi surface topology, comparing observed band structure to theory, and making connections with bulk measurements.

1:03PM Y31.00008 $a_1g$-$e_g$ splitting and the small Fermi surface pockets in Na$_x$CoO$_2$. MICHELLE JOHANNES, DEVINA PILLAY, IGOR MAZIN, Naval Research Laboratory, Washington D.C., OLE ANDERSEN, Max Planck Institute for Fekorporforschung, Stuttgart, Germany — Because DFT calculations and ARPES experiments disagree on the existence of six small Fermi surface pockets in NaCoO$_2$, it has been suggested that correlation effects neglected by the LDA may be responsible for suppressing the eg-derived pockets. Recent DMFT work has shown that such suppression is only possible if the position of the eg band is lower than that of the a1g band, prior to correlation effects. Here we show that the energy difference between band positions, $\Delta = e_{g1}-a_{1g}$ strongly depends on Na content, Na positions, and on whether bands stem from the surface or bulk. We show that the Coulomb of the Na ions is enough to shift the a1g band beneath the eg band, even though simple crystal field arguments would suggest the opposite.

1:15PM Y31.00009 Resonant Ultrasound Studies of Quasi-2D Na$_x$CoO$_2$ (0.7 < x < 0.77). TIMOTHY CABLE, VEERKE KEPPING, Department of Materials Science and Engineering, The University of Tennessee, RONGYING JIN, Materials Science and Technology Division, Oak Ridge National Laboratory — Cobalt-based oxides have been shown to represent a new paradigm for a good thermoelectric material. These materials violate all of the traditional guidelines to help identify a potentially good thermoelectric material. In order to obtain a better understanding of its physical properties, we have initiated the synthesis of layered Na$_x$CoO$_2$, and started a study of the elastic properties of these materials using Resonant Ultrasound Spectroscopy (RUS). In this work, we discuss our results for sodium cobaltate compounds with 0.7 < x < 0.77. Single crystals were successfully grown in a floating-zone furnace, and the elastic constants have been measured as a function of temperature (5-300K) and in magnetic fields up to 5 Tesla. The resulting plots of elasticity vs. temperature clearly reflect a transition below 50 K, which is believed to be associated with rearrangement of the Na-atoms between the Co$_2$ planes.

1:27PM Y31.00010 Thermo-magnetic effect of cobalt oxides. WATARU KOSHIBAE, Sendai National College of Technology, SADAMICHI MAEKAWA, IMR, Tohoku University, CREST-JST — The cobalt oxide, Na$_2$CoO$_2$, shows not only a large thermoelectric response but also an anomalous high-temperature Hall effect: The Hall coefficient increases linearly as a function of temperature and the magnitude comes to no fewer than 8 times as large as the expected Drude value. On the electron system with the large thermopower and the large Hall coefficient, an interesting behavior is expected in the response to a magnetic field upon a temperature gradient. We have studied the electronic state of the cobalt oxide and found that the electronic structure reflects the nature of the kagomé lattice hidden in the Co$_2$O$_3$ layer. We will show the importance of the hidden kagomé lattice structure in the emergence of the anomalous Hall effect and the close relationship between the Hall and Nernst coefficients.

1:39PM Y31.00011 Nodal $d+id$ pairing and topological phases on the triangular lattice: unconventional superconducting state of Na$_x$CoO$_2$ $\cdot$ $y$H$_2$O. SEN ZHOU, Florida State University, ZIQIANG WANG, Boston College — We show that the finite angular momentum pairing on the triangular lattice has point nodes in the complex gap function. A topological quantum phase transition takes place through a gapless critical state at a specific carrier density $x_c$ where the normal state Fermi surface crosses these isolated nodes. For spin singlet pairing, we show that the second nearest neighbor $d+id$ pairing is the dominate superconducting channel. The gapless critical state appears at $x_c \approx 0.25$ for the sodium cobaltates. It has six Dirac points and is topologically nontrivial with a $T^3$ spin rotation below $T_c$. This theory provides a consistent explanation for the unconventional superconducting state of Na$_x$CoO$_2$ $\cdot$ $y$H$_2$O.

1:51PM Y31.00012 Unusual Muon Spin Relaxation in Hydrated Cobaltite Superconductors. SCOTT L. STUBBS, JESS H. BREWER, Univ. of British Columbia, JUN SUGIYAMA, YUTAKA Y. IKEKO, Toyota CRDL, PETER L. RUSSO, TRIUMF, EDUARDO J. ANSALDO, Univ. of Saskatchewan, KIM H. CHOW, Univ. of Alberta, HIROTO OHTA, KAZUYOSHI YOSHIMURA, Dept. of Chemistry, Kyoto Univ. — Muon spin relaxation ($\mu^+$SR) was studied in zero (ZF) and weak magnetic field (TF) in Na$_x$(H$_2$O)$_3$CoO$_2$ $\cdot$ $y$H$_2$O and its deuterated analog. In ZF, the muon relaxes (surprisingly) faster for the deuterated sample. Detectable effects of superconductivity are also surprisingly subtle in both cases.

Friday, March 14, 2008 11:15AM - 2:15PM –
Session Y32 DCOMP DMP GMAG: Focus Session: Theory and Simulations of Magnetism II
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Determining the magnetic ground state of systems exhibiting metastable states close to the ground state. This freedom of the method might cause an ambiguity in chirality. For the linear and the isosceles Cr trimers we obtain collinear antiferromagnetic ground states. We also address the issue of choosing the reference state equations. In case of an equilateral Cr trimer we show that the Dzialoshinsky-Moriya interactions lift the degeneracy of the $120^\circ$ state.

The magnetic ground-state of the trimers are found as the solution of the Landau-Lifshitz-Gilbert equations. In addition, we show that the inclusion of fourth-order terms into the FLAPW code FLEUR which can cope with this challenge. We show by first-principles calculations based on the vector-spin density formulation of the density-functional theory (DFT) that that there are circumstances where the DM interaction is indeed sufficiently strong to compete with the interactions that favor collinear spin alignment causing magnetic phases of unique handedness e.g., homochiral magnetic phases such as a left rotation cycloidal spiral in Mn on W(110) [M. Bode et al., Nature 447, 190 (2007)] or favoring magnetic domain-walls with unique turning sense.

Supported by DFG-SPP-1143, DFG-ESF-SANMAG and DFG-BI 823/1

11:15 AM Y32.00001 Homochiral magnetic structures at surfaces. STEFAN BLUGEL, Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — Electrons propagating in the vicinity of inversion asymmetric environments such as surfaces, interfaces, ultrathin films or nanostructures can give rise to an important antisymmetric exchange interaction, known as Dzyaloshinsky-Moriya (DM) interaction. Although this interaction, favoring spatially rotating spin structures, is in principle known for about 50 years, its consequences for the magnetic structure in low-dimensional magnets remained nearly unexplored and has been basically overlooked the past 20 years. Theoretical models considering isotropic exchange, magnetic anisotropy and the DM interaction display a rich phase diagram of complex magnetic phases on different length scales depending on the strength of the different contributions. Today, it is unknown how large is the strength of the DM interaction. Is this just a small perturbation to the collinear uniaxial ferro- or antiferromagnetic state, determined by exchange and magnetic anisotropy or is it strong enough to create new phases which had been overlooked? Surprisingly little first-principles calculations deal with the DM interaction. There might be several reasons for this: The investigation requires the treatment of non-collinear magnetism together with spin-orbit interactions of large magnetic structures in low-symmetry situations. We developed a perturbative strategy implemented into the FLAPW code FLEUR which can cope with this challenge. We show by first-principles calculations based on the vector-spin density formulation of the density-functional theory (DFT) that that there are circumstances where the DM interaction is indeed sufficiently strong to compete with the interactions that favor collinear spin alignment causing magnetic phases of unique handedness e.g., homochiral magnetic phases such as a left rotation cycloidal spiral in Mn on W(110) [M. Bode et al., Nature 447, 190 (2007)] or favoring magnetic domain-walls with unique turning sense.

1Supported by DFG-SPP-1143, DFG-ESF-SANMAG and DFG-BI 823/1

11:51 AM Y32.00002 First-principles Calculation of Magnetic Anisotropy of a Single Atom on a Surface. CHIUNG-YUAN LIN, National Chiao Tung University, BARBARA JONES, IBM Almaden Research Center — Recent progress on scanning tunneling microscopy has made it possible to position (in atomic-scale accuracy) and probe single magnetic atom on material surfaces. Targeting the fabrication of a single-atom data storage bit, we perform first-principles calculations of single magnetic atoms (Fe and Mn) on a surface. Structure relaxation determines the binding structures of the magnetic atoms to its surroundings. Charge analysis indicates that the magnetic atoms form polar covalent bonds with the surface. Spin density is found to spread up to 4 Å from the magnetic atom, which is qualitatively similar to that reported in DFT calculations of molecular magnets. Total energies with spin-orbit interaction included are calculated in different spin orientations, and are compared to the anisotropy axes measured in the experiments.

Supported by Stanford University, Center for Probing the Nanoscale

12:03 PM Y32.00003 First-principles study on the surface half-metallicity of CaC in the zincblende structure. KAILUN YAO, GUOYING GAO, ZULI LIU, Huazhong University of Science and Technology — We investigate the electronic structure and the surface half-metallicity of CaC in the zincblende structure by using the first-principles full-potential linearized augmented plane-wave (FPLAPW) method. It is found that the (1 1 0) surface preserves the half-metallic character of the bulk, while in the case of the (0 0 1) surfaces including the Ca-terminated and C-terminated surfaces the surface states destroy the half-metallicity.

This work was supported by the National Natural Science Foundation of China under Grant Nos. 10574047, 10574048 and 20490210. It was also supported by National 973 project under grant No. 2006CB921600.

12:15 PM Y32.00004 Finite Hubbard clusters with large spin polarization. ERIK NIELSEN, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, R.N. BHATT, Department of Electrical Engineering, Princeton University; Princeton Center for Theoretical Physics, Princeton, NJ 08544 — A generalized Hubbard model can be used to characterize hydrogenic impurities in semiconductors. It has been shown that the ground state spin of such impurity clusters is very sensitive to a cluster’s electron number and geometry [1]. An understanding of how these factors affect cluster magnetization is particularly relevant in light of the current ability to position phosphorus donors with nanometer accuracy within bulk silicon [2]. We present numerical results for two-dimensional clusters showing the effect of geometry and electron-hole asymmetry present in real systems of hydrogenic donors. We also consider the robustness of high-spin cluster ground states to perturbations of site position, and discuss the general features of clusters found to possess a high-spin ground state, in particular the fully spin-polarized state.


Supported by NSF-MRSEC (DMR-0213706).

12:27 PM Y32.00005 Magnetic ground state of small nanoparticles: Cr trimers on Au(111). BALAZS UJFALUSSY, Research Institute for Solid State Physics — The development of scanning tunneling microscopy (STM) and the ability to build clusters with well-controlled structures permit the study of various effects induced by local interactions within magnetic nanoclusters. However, for a clear interpretation of experimental results, first principles studies are often required, even when they are sometimes too demanding. In this talk we show a new way to map the energy of supported magnetic nanoparticles obtained from first principles calculations onto a classical spin Hamiltonian. The half-filled valence configuration of Cr yields a large magnetic moment and strong antiferromagnetic inter-atomic bonding leads in turn to magnetic frustration and complex spin phenomena. The simplest system exhibiting such properties is a trimer. The electronic structure of the Cr trimers are calculated by means of a fully relativistic Green’s function embedding method. The relativistic treatment of the electronic structure leads to a proper account of spin-orbit coupling giving rise to tensorial exchange interactions and magnetic anisotropies influencing the formation of non-collinear ground states. In addition, we show that the inclusion of fourth-order terms into the spin-model largely enhance the accuracy of the mapping. The magnetic ground-state of the trimers are found as the solution of the Landau-Lifshitz-Gilbert equations. In case of an equilateral Cr trimer we show that the Dzialoshinsky-Moriya interactions lift the degeneracy of the $120^\circ$ Néel states with different chirality. For the linear and the isosceles Cr trimers we show collinear antiferromagnetic ground states. We also address the issue of choosing the reference state inherent to methods based on the magnetic force theorem in the context to the equilateral Cr trimer. This freedom of the method might cause an ambiguity in determining the magnetic ground state of systems exhibiting metastable states close to the ground state.

Work supported in part by the Division of Material Science and Engineering US-DOE and by the Hungarian government (contracts OTKA 68312 and F68726).
2:03PM Y32.00006 A Numerical Method to Study Highly Correlated Nanostructures: The Logarithmic Discretization Embedded Cluster Approximation, E. ANDA, G. CHIAPPE, C. BUSser, M. DAVIDOVICH, G. MARTINS, F. H-MEISNER, E. DAGOTTO, Oak蘭d University — A numerical algorithm to study transport properties of highly correlated local structures is proposed. The method, dubbed the Logarithmic Discretization Embedded Cluster Approximation (LDECA), consists of diagonalizing a finite cluster containing the many-body terms of the Hamiltonian and embedding it into the rest of the system, combined with Wilson’s ideas of a logarithmic discretization of the representation of the Hamiltonian. LDECA’s rapid convergence eliminates finite-size effects commonly present in the embedding cluster approximation (ECA) method. The physics associated with both one embedded dot and a string of two dots side-coupled to leads is discussed. In the former case, our results accurately agree with Bethe ansatz (BA) data, while in the latter, the results are framed in the conceptual background of a two-stage Kondo problem. A diagrammatic expansion provides the theoretical foundation for the method. It is argued that LDECA allows for the study of complex problems that are beyond the reach of currently available numerical methods.

1:15PM Y32.00007 Coulomb and spin-orbit effects in quantum dot molecules under harmonic fields, LILIA MEZA-MONTES, Instituto de Fisica B. Universidad Autonoma de Puebla, Mexico, AREZKY H. RODRIGUEZ, Universidad Autonoma de la Ciudad de Mexico, SERGIO E. ULLOA, Dept. of Phys. and Astron. CMS- NQPI Ohio University — The time evolution of a two-electron quantum dot molecule under strong harmonic electric fields is studied. The wave function is determined in terms of the single-electron orbitals using the Floquet approach. We pay particular attention to the evolution of the spin states of the system, as the surface inversion asymmetry (Rashba-type) and bulk inversion asymmetry (Dresselhaus-type) spin-orbit effects are known to introduce spin mixing. We also study the role of a perpendicular magnetic field, which is shown to have dramatic effects on the dynamics. We present an analysis of the physical behavior of the system in terms of the quasi-energy spectrum, and study the time evolution of the occupation probabilities of the dots. Conditions for singlet-triplet mixing, similar to the spin-flips observed in the single-electron case, are analyzed. These results are relevant for applications in spin-controlled devices.

1:27PM Y32.00008 Electron Transport in Nanogranular Ferromagnets, IGOR BELOBORODOV, University of Chicago, ANDREAS GLATZ, VALERII VINOKUR, Argonne National Laboratory — I will discuss electronic transport properties of ferromagnetic nanoparticle arrays and nanodomain materials near the Curie temperature in the limit of weak coupling between the grains. The conductivity is calculated in the Ohmic and non-Ohmic regimes and the magnetoresistance jump in the resistivity at the transition temperature is estimated. The results are applicable for many emerging materials, including artificially self-assembled nanoparticle arrays and a certain class of manganites, where localization effects within the clusters can be neglected.

1:39PM Y32.00009 Inverse band structure optimization of (InAs)/(GaAs) (001) nanostructures for thermophotovoltaics, PAULO PIQUINI, PETER GRAF, ALEX ZUNGER, National Renewable Energy Laboratory — Thermophotovoltaic materials converting black-body thermal radiation to electricity often require conversion efficiency for materials with direct band gaps of 0.6 eV. Random In$_{53}$Ga$_{47}$As alloy lattice matched to InP have a gap around 0.76 eV, too big for this application. Therefore, difficult to grow lattice-mismatched In-rich InGaAs alloys have been attempted in the past. Here we suggest to use (InAs)$_n$/(GaAs)$_m$ ordered superlattices (rather than random), lattice matched to InP substrates. Using empirical pseudopotential calculations and genetic algorithm methods we look for the sequence of InAs and GaAs pure layers that simultaneously lead to a target band gap of 0.6 eV and has a minimum in-plane stress (strain balance condition). Further, since for (InAs)$_n$ layers with $n>5$ the two-dimensional growth is unstable and SK quantum dots are seen to form, we restrict the value for the period of the InAs layers to be always lower than 5.

1:51PM Y32.00010 Spin-blockade in a Hubbard chain with spin-dependent impurities, CHANG-QIN WU, YAO YAO, Department of Physics, Fudan University, Shanghai, CHINA — We investigate the spin/charge transport in a one-dimensional strongly-correlated system using adaptive time-dependent density matrix renormalization group method. The model we consider is a non-half-filled Hubbard chain with spin-dependent impurities, which is found to display the blockade of spin current while little influence on charge current. We have considered (1) the spread of a wave packet of both spin and charge in the Hubbard chain and (2) the spin and charge currents induced by a spin-dependent voltage bias that is applied to the ideal leads attached at the ends of this Hubbard chain. It is found that the spin-charge separation plays a key role in the spin-blockade and a large on-site repulsion $U$ is required for more effective utilization of this phenomenon in some spin-related devices, like spin memory.

2:03PM Y32.00011 Signature of hyperfine interaction through current properties in quantum dots, ERNESTO COTA, FERNANDO ROJAS, Centro de Ciencias de la Materia Condensada, Universidad Nacional Autonoma de Mexico, SERGIO E. ULLOA, Ohio University — Several experiments have been carried out to observe and control spin properties of electrons in quantum dots subject to the hyperfine interaction due to nuclear spins. In this work, we study the manifestation of the hyperfine interaction through current calculations in one and two quantum dots. We use the density matrix master equation approach in the stationary regime taking into account an external magnetic field and the nuclear magnetic field in the quasistatic approximation characterized by the statistical fluctuations of the components of the nuclear field. As a first step, we study the case of a single quantum dot with one orbital. We study in detail the effects on the current of the hyperfine interaction, temperature and external magnetic field and we find that it is possible to obtain information on the hyperfine interaction directly from the differential conductance. We extend the model to study a double quantum dot with one and two electrons, including tunneling and exchange interactions, where the signature of the hyperfine interaction is more involved.

Friday, March 14, 2008 11:15AM - 2:03PM — Session Y33 GMAG FIAP DMP: Focus Session: Diluted Magnetic Oxides Morial Convention Center 224

11:15AM Y33.00001 Room-Temperature Electron Spin Dynamics in Free-Standing ZnO Quantum Dots, DAN CAMELIN, University of Washington — No abstract available.

3Partially supported by CONACyT-Mexico and NSF-WMN.

1Work supported by NSF of China.
11:51 AM  Y33.00002 Insulator-ferromagnetic metal transition in anatase Fe:TiO$_2$. ENJU SAKAI, The University of Tokyo, YASUSHI HIROSE, KAST, TARO HITSUGI, TOSHIHIRO SHIMADA, TETSUYA HASEGAWA, The University of Tokyo, KAST — Local Fe valence states in Fe-doped anatase TiO$_2$ (Fe:TiO$_2$) were investigated in relation with transport and magnetic properties. Anatase Fe:TiO$_2$ films were deposited on LaAlO$_3$ (100) substrates by pulsed laser deposition technique. Amounts of oxygen vacancies in the films were controlled by varying partial oxygen pressure during deposition ($P_{O_2}$). Magnetic and transport properties of the synthesized Fe:TiO$_2$ films measured by SQUID and conventional four-probe measurements. An insulator-ferromagnetic metal transition was clearly observed between $P_{O_2} = 1 \times 10^{-6}$ and $3 \times 10^{-6}$ Torr. X-ray photoemission spectroscopy (XPS) measurements have revealed that the local Fe valence state changes from 3+ to 2+, accompanied with the insulator-ferromagnetic metal transition. These results strongly suggest that carriers bound to Fe-oxygen vacancy pairs form magnetic polarons, and that mutual overlap of magnetic polarons triggers the insulator to ferromagnetic metal transition in Fe:TiO$_2$.

12:03PM Y33.00003 Insights into magnetically doped semiconductors from soft x-rays$^1$. D.J. KEAVNEY, Argonne National Laboratory, D.B. BUCHHOLZ, Northwestern University, Q. MA, Northwestern University Synchrotron Research Center, R. CHANG, Northwestern University, T.C. DROUBAY, T.C. KASPAR, S. CHAMBERS, Pacific Northwest National Laboratory — Soft x-ray absorption and dichroism provide a crucial test of the intrinsic nature of magnetism in doped semiconductor. Experiments on Mn, Co, and Cu-doped ZnO reveal that the magnetic dopants have primarily paramagnetic field and temperature dependence regardless of whether the bulk behavior is ferromagnetic. In PLD-grown ferromagnetic Cu:ZnO, no zero-field dichroism is detected at the Cu L, O K, or Zn L edges. In MOVCD-grown Co:ZnO, we find a small remanent signal that is consistent with bulk magnetization measurements of $\sim 0.04 \mu_\text{B}/\text{Co ion}$, however the signal is insufficient to rule out metallic Co as its origin. These results suggest that the origins of ferromagnetism in doped oxides may be unrelated to the presence of magnetic dopants.

$^1$Use of the Advanced Photon Source was supported by the U. S. DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

12:15PM Y33.00004 Structural, Magnetic and Transport Properties of a New Class of Ferromagnetic Semiconductors/Metals: (Ba, Sr)$_2$M$_{2+x}$Ru$_{1-x}$O$_{11}$ (M = Fe, Co)$.^2$ LARYSA SHLYK, LANCE DE LONG, SERGIY KRYUKOV, Dept. of Physics and Astronomy, University of Kentucky, BARBARA SCHÜPP-NIEWA, RAINER NIEWA, Department Chemie, Technische Universität München — Single crystals (mm size) of (Ba, Sr)$_2$Fe$_{2+x}$Ru$_{1-x}$O$_{11}$ and (Ba, Sr)$_2$Co$_{2+x}$Ru$_{1-x}$O$_{11}$ were grown for the first time. X-ray refinements confirmed a hexagonal space group (P6$_3$/mmc, No. 194) with two crystallographic sites having mixed Ru and Fe/Co occupation, and one site occupied exclusively by the 3d species. Structural parameters and charge balance suggest oxidation states Co$^{2+}$ and mixed Ru$^{3+}$/Ru$^{4+}$ in the Co compound, and mixed Fe$^{2+}$/Fe$^{3+}$ and Ru$^{4+}$/Ru$^{5+}$ in the Fe compound. The physical properties of these single crystals are sensitive to site disorder among the transition metal ions. Magnetic and transport measurements show the Co-bearing barium ferrite is a ferromagnetic metal below 105 K. In contrast, Fe-bearing barium and strontium compounds exhibit long-range ferromagnetic order at temperatures above 400 K, and narrow-gap semiconductor properties that include a large anomalous Hall conductance, low resistivity, and high carrier concentration. These characteristics make the Fe-bearing materials promising new candidates for spintronic applications.

$^2$Research was supported by U.S. DoE Grant DE-FG02-97ER45653.

12:27PM Y33.00005 Spin coherence of electrons in singly-charged quantum dots. DMITRI YAKOVLEV, Technical University Dortmund — We present experimental and theoretical study on electron spin coherence in ensemble of n-type doped InGaAs/GaAs quantum dots containing one electron per dot. A pump-probe time-resolved Faraday rotation technique is exploited. Long-lived spin precession of resident electrons in external magnetic fields is observed with the dephasing time of spin ensemble exceeding 6 ns. Rabi oscillations of the Faraday rotation amplitude have been detected confirming the suggested model of generation electron coherent via excitation of coherent superposition of the spin state and the resident electron [1]. We show that the ensemble dephasing can be overcome by using a periodic train of light pulses to synchronize the phases of the precessing spins. This mode-locking leads to constructive interference of contributions to Faraday rotation, and presents potential applications based on robust quantum coherence within an ensemble of dots [2, 3]. Under these experimental conditions spins of the dots nuclei are aligned in a way that all dots in the ensemble contribute to the coherent signal with a potential to focus the electron Larmor frequencies in the ensemble to a single mode [4]. The used optical technique allows to recover the coherence time of a single quantum dot. The measured spin coherence time is 3 microseconds, which is four orders of magnitude longer than the ensemble dephasing time of 400 picoseconds. This work is done in collaboration with A. Greilich, I. A. Yugova, R. Oulton, M. Bayer, A. Shabaev, Al. Efros, D. Reuter and A. D. Wieck.


1:03PM Y33.00006 Impurity-Ion pair induced high-temperature ferromagnetism in Co-doped ZnO. STEFANO SANTIVO, CHAITANYA DAS PEMMARAJU, RUAIRI HANAFIN, THOMAS ARCHER, School of Physics and CRANN, Trinity College Dublin, HANS BENJAMIN BRAUN, School of Physics, University College Dublin — Magnetic 3d-ions doped into wide-gap oxides show signature of room temperature ferromagnetism, although their concentration is two orders of magnitude smaller than that of conventional magnets. The prototype of these exceptional materials is Co-doped ZnO, for which an explanation for the room temperature ferromagnetism is still elusive. Here we demonstrate that magnetism originates from Co$^{2+}$ oxygen-vacancy pairs with a partially filled level close to the ZnO conduction band minimum. The magnetic interaction between these pairs is sufficiently long-range to cause percolation at moderate concentrations. However, magnetically correlated clusters large enough to show hysteresis at room temperature already form below the percolation threshold and explain the current experimental findings. Our work demonstrates that the magnetism in ZnO:Co is entirely governed by intrinsic defects and a phase diagram is presented. This suggests a recipe for tailoring the magnetic properties of spintronics materials by controlling their intrinsic defects.

1:15PM Y33.00007 Magnetic 3d interactions in ZnO and In$_2$O$_3$ in a band-gap corrected approach. STEPHEN LANY, H. RAEBIGER, A. ZUNGER, Natl. Renewable Energy Lab — The electronic and magnetic configuration of 3d transition metal (TM) impurities in wide-gap oxides like ZnO and In$_2$O$_3$ is misrepresented in the standard LDA and GGA approximations to density functional theory: Because the conduction band minimum lies energetically much too low, the spin-polarized impurity states wrongly occur as resonances inside the conduction band rather than as gap states. Due to spurious “charge spilling” from the TM impurity state into the host conduction band, the magnetic moment and the occupancy of the TM impurity state is incorrect, and the TM state becomes partially occupied, which is prone to cause overestimated ferromagnetic interactions. These errors in the LDA+U or GGA+U methods often applied to TM-doped states. In our band-gap corrected approach, we augment the GGA+U functional by empirical non-local external potentials (NLEP) for the $s$- and $p$-states of Oxygen and the cations. In this approach the correct spin and orbital configuration of the TM impurity-states is recovered. In the absence of additional doping, we find generally short-ranged magnetic interactions, and pronounced Jahn-Teller effects in case of partially occupied gap states. Additional electron-doping can lead to more long-range ferromagnetic interactions for those TM-dopants that have unoccupied d-states which hybridize strongly with the conduction band.
1:27PM Y33.00008 Study of the anomalous Hall effect, magnetoresistance, and magnetic anisotropy in ZnO:Co and ZnO:Mn thin films. Z. YANG, Z. ZUO, Y. PU, M. BIASINI, W. BEYERMANN, J. SHI, J. LIU, QUANTUM STRUCTURES LABORATORY, DEPT OF ELECTR ENGR, UNIV OF CALIFORNIA, RIVERSIDE, CA TEAM — ZnO-based diluted magnetic semiconductor (DMS) materials have attracted much attention in these years due to the theoretical prediction of above room-temperature ferromagnetism. So far, most of the experiments were focused to the study of the magnetization of the ZnO DMS materials. However, the magnetization study, by only providing a global information on the moment of the material, cannot distinguish the intrinsic magnetic properties from the extrinsic contributions. The ZnO thin films were grown on sapphire substrates by molecular-beam epitaxy. The Co- and Mn-implantations were performed on the as-grown ZnO samples with different free carrier concentrations. Anomalous Hall effect (AHE) and magnetoresistance measurements were performed on the ZnO:Co and ZnO:Mn thin films. AHE hysteresis loops were observed in both ZnO:Co and ZnO:Mn thin films, which confirm the intrinsic ferromagnetism in both films. However, the AHE hysteresis loops are distinctly weaker than the magnetization hysteresis loops (\(M - H\)) measured by SQUID. Therefore we conclude that both intrinsic and extrinsic ferromagnetism co-exist in the samples.

1:39PM Y33.00009 Influence of oxygen partial pressure on structural, transport and magnetic properties of Co doped TiO2 films. BAKHTYAR ALI, Department of Physics and Astronomy, University of Delaware, Newark DE, 19716, USA, ABDUL RUMAIZ, ARIF OZBAY, S. ISMAT SHAH, EDMUND NOWAK — Crystal structure, transport and magnetic properties of Co doped TiO2 laser ablated thin films are investigated and are found to have a strong dependence on the oxygen partial pressure. X-ray diffraction reveals the presence of mixed phase material containing anatase and rutile. However, these phases intertransform with the change in the oxygen partial pressure in the chamber during the growth of the films under the same temperature and other growth conditions. Electrical conductivity enhances as more oxygen vacancies are created. Concomitantly, the magnetization increases with increased vacancy concentration. The electrical transport data is suggesting that the conduction is dominated by polarons. The activation energies obtained are in the range from 100 to 150meV, typical for semiconducting oxides. APS Membership: Pending

Friday, March 14, 2008 11:15AM - 2:15PM Session Y36 FIAP: Focus Session: Artificial Neurons Morial Convention Center 228

11:15AM Y36.00001 Understanding the dynamical control of animal movement. DONALD EDWARDS, Georgia State University — Over the last 50 years, neurophysiologists have described many neural circuits that transform sensory input into motor commands, while biomechanicians and behavioral biologists have described many patterns of animal movement that occur in response to sensory input. Attempts to link these two have been frustrated by our technical inability to record from the necessary neurons in a freely behaving animal. As a result, we don’t know how these neural circuits and patterns are structured, or how they change with context change or time-scale. To address this problem, we have developed a software package, AnimatLab (www.AnimatLab.com), that enables users to reconstruct an animal’s body and its relevant neural circuits, to link them at the sensory and motor ends, and through simulation, to test their ability to reproduce appropriate patterns of the animal’s movements in a simulated Newtonian world. A Windows-based program, AnimatLab consists of a neural editor, a body editor, a world editor, stimulus and recording facilities, neural and physics engines, and an interactive 3-D graphical display. We have used AnimatLab to study three patterns of behavior: the grasshopper jump, crayfish escape, and crayfish leg movements used in postural control, walking, reaching and grasping. In each instance, the simulation helped identify constraints on both nervous function and biomechanical performance that have provided the basis for new experiments. Colleagues elsewhere have begun to use AnimatLab to study control of paw movements in cats and postural control in humans. We have also used AnimatLab simulations to guide the development of an autonomous hexapod robot in which the neural control circuitry is downloaded to the robot from the test computer.

11:51AM Y36.00002 Biomechanical Analysis of Locust Jumping in a Physically Realistic Virtual Environment. DAVID COFER, GENNADY Cymbalyuk, Georgia State University, WILLIAM HEITLER, Univ. of St. Andrews, DONALD EDWARDS, Georgia State University — The biomechanical and neural components that underlie locust jumping have been extensively studied. Previous research suggested that jump energy is stored primarily in the extensor apodeme, and in a band of cuticle called the semi-lunar process (SLP). As it has thus far proven impossible to test this hypothesis directly, after the locust has been killed and placed in a dissecting pan, we have been able to test whether the energy stored in the SLP has a significant impact on the jump. To address problems such as this we have developed a software toolkit, AnimatLab, which allows researchers to build and test virtual organisms. We used this software to build a virtual locust, and then asked how the SLP is utilized during jumping. The results show that without the SLP the jump distance was reduced by almost half. Further, the simulations were also able to show that loss of the SLP had a significant impact on the final phase of the jump. We are currently working on postural control mechanisms for targeted jumping in locust.

12:03PM Y36.00003 Design of real-time locomotion generator with map-based neuronal models. NIKOLAI RULKOV, UCSO, JOSEPH AYERS, NEU, MARK HUNT, Ariel Inc. — We are developing an electronic nervous system for a biomimetic robot based on an established neurobiological model system, the Sea Lamprey. Undulatory locomotion of the lamprey is coordinated by a concatenated network of over 100 segmental central pattern generators (CPGs). To achieve real time operation in a DSP chip, we are using simple phenomenological models of neurons and synapses based on the dynamics of nonlinear maps. CPG networks based on known neuronal circuitry have replicated main properties of the dynamical behavior of the animal model. The results of numerical studies of the neuronal activity coordinating various swimming patterns in the reduced model of the CPG are considered. Both ascending and descending connections between segmental CPGs can mediate both forward and backward propagating flexion waves based on anterior or posterior bias by descending premotor commands. Bilaterally asymmetric biases of descending commands can mediate turning. The CPG outputs control 5 shape memory alloy actuators on each side to generate coordinated undulations. Two dorsal and ventral pitch actuators control the angle between the hull and undulator to control dive and climb. Descending commands are modulated by an analog compass, inclinometers, accelerometers and other sensory feedback to mediate hovering by the vehicle on a sonar beacon.

1:51PM Y33.00010 Spin-polarized tunneling study of the room temperature spin filter CoFe2O4. ANA RAMOS, JEAN-BAPTISTE MOUSSY, DSM/DRECAM/SCPSI, CEA Saclay, France, RICHARD MATTANA, Unité Mixte de Physique, CNRS/Thales, Palaiseau, France, FREDERIC PETROFF, Unité Mixte de Physique, CNRS/Thales, Palaiseau, France, TIFFANY SANTOS, Argonne National Laboratory, Argonne, IL, USA, GUO-XING MIAO, JAGADEESH MOODERA, Francis Bitter Magnet Lab, MIT, Cambridge, MA, USA — The spin filter effect has the potential of generating highly spin-polarized electron currents across the spin selective transport of electrons across a ferromagnetic tunnel barrier. In this work, we investigate the spin-polarized tunneling characteristics of cobalt ferrite (CoFe2O4), which we show is a room temperature spin filter. Tunnel junctions containing epitaxial CoFe2O4(111) tunnel barriers have been grown by oxygen plasma-assisted molecular beam epitaxy. Their structural, chemical and magnetic properties have previously been optimized by a number of in situ and ex situ methods, we focus on the spin-polarized tunneling in the CoFe2O4-based systems using different measurement techniques. Following the demonstration of spin filtering by TMR measurements, both at low temperature and at room temperature, we further investigate the spin filter characteristics of CoFe2O4 in detail. In particular, we pay special attention to the influence of defects on the spin polarization, as well as the role of different spin-detecting electrodes.

*Funded by CNANO Ile de France and the MIT-France Program*
12:15PM Y36.00004 Genesis and synchronizion properties of fast neural oscillations\textsuperscript{1}, MAXIM BAZHENOV, Salk Institute, NIKOLAI RULKOV, UCSD — Fast neural network oscillations in gamma (30-80 Hz) range are associated with attentiveness and sensory perception and have strong relation to both cognitive processing and temporal binding of sensory stimuli. These oscillations are found in different brain systems including cerebral cortex, hippocampus and olfactory bulb. Cortical gamma oscillations may become synchronized within 1-2 msec over distances up to a few millimeters. In this study we used computational network models to analyze basic synaptic mechanisms and synchronization properties of fast neural oscillations. Using the network models of synaptically coupled pyramidal neurons (up to 500,000 cells) and fast spiking interneurons (up to 125,000 cells) we found that the strength of feedback inhibition determined the network synchronization state: either global network oscillations with near zero phase lag between remote sites or waves of gamma activity propagating through the network. Long-range excitatory connections between pyramidal cells were not required for long-range synchronization. The model predicts that local inhibitory circuits can mediate global network synchronization with phase delays being much smaller than activity propagation time between remote network sites.

\textsuperscript{1}Supported by NIDCD.

12:27PM Y36.00005 Periodic vs. Transient Estimation of Phase Response Curves\textsuperscript{1}, JIANXIA CUI, Georgia Institute of Technology, SRISAIRAM ACHUTHAN, CARMEN CANAVIER, LSU Health Sciences Center, ROBERT BUTERA, Georgia Institute of Technology — Phase response curves (PRCs) for a single neuron are often used to predict the synchrony of mutually coupled neurons. Previous theoretical work on pulse coupled oscillators used single pulse perturbations. We propose an alternate method in which functional PRCs (FPRCs) are generated using a train of pulses applied at a fixed delay after a spike. Experimental FPRCs in \textit{Aplysia} pacemaker neurons were different from single pulse PRCs because of adaptation. Adaptation was incorporated by plotting the effective period, observed just after the pulse train is terminated, as a function of the entrained period during the pulse train. The effective intrinsic period was used iteratively in the prediction method instead of the unperturbed intrinsic period. Incorporating adaptation improved the accuracy of prediction of phase-locked modes in a model network of adapting oscillators characterized by both single pulse and multiple pulse PRCs compared to those characterized by single pulse PRCs alone.

\textsuperscript{1}Supported by NIH NS45281.

12:39PM Y36.00006 Homoclinic Spike adding in a neuronal model in the presence of noise\textsuperscript{1}, IBINYINKA FUWAPE, ALEXANDER NEIMAN, Ohio University, Athens, Ohio, ANDREY SHILNIKOV, Georgia State University, Atlanta — We study the influence of noise on a spike adding transitions within the bursting activity in a Hodgkin-Huxley-type model of the leech heart interneuron. Spike adding in this model occurs via homoclinic bifurcation of a saddle periodic orbit. Although narrow chaotic regions are observed near bifurcation transition, overall bursting dynamics is regular and is characterized by a constant number of spikes per burst. Experimental studies, however, show variability of bursting patterns whereby number of spikes per burst varies randomly. Thus, introduction of external synaptic noise is a necessary step to account for variability of burst durations observed experimentally. We show that near every such transition the neuron is highly sensitive to random perturbations that lead to and enhance broadly the regions of chaotic dynamics of the cell. For each spike adding transitions there is a critical noise level beyond which the dynamics of the neuron becomes chaotic throughout the entire region of the parameter transition. Noise-induced chaotic dynamics is characterized in terms of the Lyapunov exponents and the Shannon entropy and reflects variability of firing patterns with various numbers of spikes per burst, traversing wide range of the neuron’s parameters.

12:51PM Y36.00007 Adaptive Neurotechnology for Making Neural Circuits Functional\textsuperscript{1}, RANU JUNG, Arizona State University, Center for Adaptive Neural Systems, Ira A. Fulton School of Engineering — Two of the most important trends in recent technological developments are that technology is increasingly integrated with biological systems and that it is increasingly adaptive in its capabilities. Neuroprosthetic systems that provide lost sensorimotor function after a neural disability offer a platform to investigate this interplay between biological and engineered systems. Adaptive neurotechnology (hardware and software) could be designed to be biomimetic, guided by the physical and programmatic constraints observed in biological systems, and allow for real-time learning, stability, and error correction. An example will present biomimetic neural-network hardware that can be interfaced with the isolated spinal cord of a lower vertebrate to allow phase-locked real-time neural control. Another will present adaptive neural network control algorithms for functional electrical stimulation of the peripheral nervous system to provide desired movements of paralyzed limbs in rodents or people. Ultimately, the frontier lies in being able to utilize the adaptive neurotechnology to promote neuroplasticity in the living system on a long-time scale under co-adaptive conditions.

1:27PM Y36.00008 Investigating the Dynamics of Functional Brain Networks with MRI, SHELLA KEILHOLZ, Emory University, WAQAS MAJEED, Georgia Institute of Technology — Functional Magnetic Resonance Imaging (fMRI) is sensitive to changes in blood oxygenation levels. While fMRI has traditionally mapped changes in these levels that localize to brain areas activated by an external stimulus, recent work has focused on detecting correlated, non-stimulus-related fluctuations in the fMRI signal throughout the brain. These fluctuations are believed to arise from spontaneous variations in local neural activity, and so correlated fluctuations from different brain areas may indicate coordinated activity. Maps of “functional connectivity” based upon these fluctuations show reproducible patterns of correlated signals. To date, research has focused on steady-state networks that persist over the entire imaging session (minutes). We are exploring the possibility of detecting changes in network activity on much shorter time scales (seconds). Preliminary analysis shows that power in the frequency band used to map functional connectivity varies over time, and that power differences correspond to changes in correlation between areas. We also detected phase differences in fluctuations that are consistent with propagating waves. These results indicate that time-varying analysis of fMRI data may provide insight into the dynamics of functional networks in the brain.

1:39PM Y36.00009 Estimating Granger causality from Fourier and wavelet transforms of time series data, MUKESH DHAMALA, Georgia State University — Experiments in many fields of science and engineering yield data in the form of time series. The Fourier and wavelet transform-based nonparametric methods are used widely to study the spectral characteristics of these time series data. We have recently extended the framework of nonparametric spectral methods to include the estimation of Granger causality spectra for assessing directional influences. We illustrate the utility of the proposed methods using artificial data and real brain data.

1:51PM Y36.00010 Anomalous Effect of Surface Diffusion on NMR Signal: Tracing the Fiber Geometry, VADYM APALKOV, NERANJAN EDIRISINGHE, GENNADY CYMBALYUK, Georgia State University — We show the strong qualitative effect of the surface diffusion channel on the echo attenuation of the NMR signal from restricted geometry, e.g., fiber system. In some range of parameters of the system the residual echo signal, which is obtained by subtracting the background value, can have anomalous behavior, which means that the echo signal has a maximum value at some finite value of the magnitude of the gradient pulses. This fact can be used to enhance the accuracy of the measurements by studying the echo signal around the maximum value. Effect described here could be also used for tuning the MRI measurements to trace fibers with particular characteristic diameters or for timely detection of changes in the diffusion coefficients and fiber diameters.
near room temperature. The hybrid system consists of a living neuron and a model neuron (or an artificial silicon neuron) interacting in the real time. Dynamic clamp is used to implement artificial ionic currents and synapses in the system (Sharp et al. 1993). Our study determines the mechanisms underlying and regulating bursting activity, based on intrinsic membrane dynamics and network interactions. The complexity of endogenous dynamics originates from the divergence of potential modes and different types of excitations and underlying patterns. Similar findings derived from the analysis of bursting, its origin and transformations are common in heart interneurons both as single cells and in the mutually inhibitory configuration.

Brains and Behavior Program at GSU

Friday, March 14, 2008 11:15AM - 2:03PM
Session Y37 FLAP: Thermodynamic and Transport Properties of Semiconductors

11:15AM Y37.0001 Impact ionization rate calculation based on GW approximation , TAKAO KOTANI, MARK VAN SCHILFGAARDE, Arizona State University — Impact ionization (IMI) means the electron-hole pair production due to high energy electron (or hole). It can control the performance of devices related to the high-field transport process. For solar cell, it was proposed to use IMI for efficient energy conversion. The IMI rate can be identified as the lifetime of an electron (imaginary part of the self-energy). Since the electron-hole pair spectrum is included in the screened Coulomb interaction W , it should be important to use full W for the calculation of the lifetime. However, to our knowledge, no such calculation has been presented for semiconductors until now. For example, Ref.[5] uses a model W . In addition, the conventional formalism of Ref.[1] contains some double-counting problem. We will show our calculation for the IMI rate based on our recently-developed quasi-particle self-consistent GW method for semiconductors. Our calculation predicts a rather smaller IMI rate. [1] A. Kuligk, N. Fitzer, and R. Redmer, PRB71, 085201(2005) [2] T.Kotani. M. van Schilfgaarde, and S.V. Faleev, PRB76, 165106 (2007)

11:27AM Y37.0002 First-principles calculations of mobilities in ultra-thin double-gate MOSFETs , OSCAR D. RESTREPO, KALMAN VARGA, Vanderbilt University, BLAIR TUTTLE, Vanderbilt University & Penn State Erie, SOKRATES T. PANTELIDES, Vanderbilt University & Oak Ridge National Laboratory — Carrier mobilities in MOSFETs are usually simulated by employing empirical scattering models. These methods do not take into account quantum mechanical effects with atomic-scale structural resolution, which are key elements to describe transport at the nano-scale. We use a novel first-principles approach to calculate mobilities in ultra-thin SOI MOSFETs [1]. For this report, we newly constructed interface models of Si(100) and amorphous SiO₂. Straining the silicon lattice results in significant increases in carrier mobility. We distinguish between the strain enhancement due to the change in velocities and the enhancement coming from the change in scattering potential. We also compare our calculations with experimental values for mobility degradation caused by radiation induced Coulomb scattering centers. We are able to quantify the contribution to the total mobility from various types of scattering centers, namely, from atomic-scale interface roughness (oxide protrusions, suboxide bonds) and scattering from point defects (dangling bonds, hydrogen). This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005)

11:39AM Y37.0003 Composition Dependence of the Hole Mobility in Dilute GaSb,As₁₋ₓ , KIRSTIN ALBERI, O.D. DUBON, U.C. Berkeley, Berkeley, CA 94720; Lawrence Berkeley National Laboratory — Carrier mobilities in MOSFETs are usually simulated by employing empirical scattering models. These methods do not take into account quantum mechanical effects with atomic-scale structural resolution, which are key elements to describe transport at the nano-scale. We use a novel first-principles approach to calculate mobilities in ultra-thin SOI MOSFETs [1]. For this report, we newly constructed interface models of Si(100) and amorphous SiO₂. Straining the silicon lattice results in significant increases in carrier mobility. We distinguish between the strain enhancement due to the change in velocities and the enhancement coming from the change in scattering potential. We also compare our calculations with experimental values for mobility degradation caused by radiation induced Coulomb scattering centers. We are able to quantify the contribution to the total mobility from various types of scattering centers, namely, from atomic-scale interface roughness (oxide protrusions, suboxide bonds) and scattering from point defects (dangling bonds, hydrogen). This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005)

11:51AM Y37.0004 Enhanced Hall coefficient in InAs/AlSb μ-Hall bars induced by ballistic electron scattering from interfacial impurities , GORAN MIHAJLOVIC, JOHN E. PEARSON, AXEL HOFFMANN, SAMUEL D. BADER, Materials Science Division, Argonne National Laboratory, MARK FIELD, GERARD J. SULLIVAN, Teledyne Scientific Company — We fabricated micrometer-sized Hall bar channels of variable width w from an InAs/AlSb quantum-well, two-dimensional electron system and studied their electrical response in perpendicular magnetic fields. For the narrowest channels (w ~ 1 μm) at low fields (<0.5 T) and 5 K, we observed that the Hall coefficient increases above its classical value. This increase persists up to temperatures of order 100 K, but its magnitude decreases with increasing channel width and disappears for w ~ 4 μm. At the same time, the longitudinal resistance decreases with increasing magnetic field. The strong negative magnetoresistance is present even for the widest channels, suggesting that boundary scattering is only partially responsible for its observation. We show that both results can be explained by a mechanism of large-angle scattering of ballistic electrons from non-ionized impurities residing at the InAs/AlSb interfaces.

Work supported by DOE under contract No. DE-AC02-06CH11357.

12:03PM Y37.0005 Superradiance And Electron Transport Through Nanosystems , LUCA CELARDO, LEV KAPLAN, Department of Physics, Tulane University, New Orleans, LA 70118 — Electron transport through a sequence of potential wells characterized by strong tunneling between them is investigated. Using the effective non hermitian Hamiltonian approach to open systems, the transition to a superradiance regime is shown to occur. The consequences of the superradiance transition on the conductance, including negative differential conductance, are investigated.

12:15PM Y37.0006 Thermal conductivity of amorphous silicon films , JOSEPH FELDMAN, XIAO LIU, Naval Research Laboratory, R. CRANDALL, National Renewable Energy Laboratory, N. BERNSTEIN, M. MEHL, D. PAPACONSTANTOPOULOS, Naval Research Laboratory — We measured the thermal conductivity of an 80 μm thick amorphous silicon film from 80K to room temperature. The amorphous silicon sample was prepared by hot-wire chemical-vapor deposition with 1 at. % hydrogen, which was found previously to contain almost no atomic tunneling states that is common in amorphous solids. The value of the thermal conductivity is about a factor of two larger than previous results. To explain this unusually large thermal conductivity, we report on a Kubo theory that makes use of a tight binding electronic structure of a 1000 atom model. We conclude that the large thermal conductivity of our film is attributed to the lack of scattering of the low frequency modes by the tunneling states. Therefore, low frequency modes can make significant contribution to heat transport even at near room temperature.
12:27PM Y37.00007 Thermoelectric properties of nanoporous Si , JOO-HYOUNG LEE, JEFFREY C. GROSSMAN, University of California-Berkeley, JOHN REED, Lawrence Livermore National Laboratory, GIULIA GALLI, University of California-Davis — Improvements in thermoelectric (TE) materials could lead to efficient solid-state energy-conversion for environmentally benign power generation and refrigeration. This realization would require a large increase to ∼ 3 in the thermoelectric figure of merit ZT at room temperature. Recent experiments have shown promise for practical applications of TE materials such as Bi$_2$Te$_3$/Sb$_2$Te$_3$ superlattices and PbS/Te/PbTe quantum dot superlattices, yielding ZT of 2.4 and 1.3 – 1.6, respectively. In addition, there have been recent attempts to use Si for TE applications due to its structural simplicity and the possibility of utilizing existing Si-based manufacturing processes. In the present work, we report theoretical studies on thermoelectric properties of Si with periodically arranged nanometer-sized pores (nanoporous Si). Specifically, we calculate the electrical conductivity, Seebeck coefficient and figure of merit of nanoporous Si for a range of configurations using a combined ab initio electronic structure calculation and Boltzmann transport approach at room temperature. The results show a substantial increase in ZT compared with that of bulk Si, similar to recent findings for ZT in Si nanowires. Approaches for increasing ZT further in this porous material will also be discussed.

12:39PM Y37.00008 ac conductivity in low dimensional structures: acoustic study, A. SUSLOV, NHMFL, Tallahassee, FL 32310, USA, I. DRICHKO, I. SMIRNOV, A. DYAKONOV, YU. GALPERIN, Joefe PTI, St Petersburg, 194021, Russia, V. VINOKUR, ANL, Argonne, IL 60439, USA — Surface acoustic waves (SAWs) were used for contactless measurements of ac conductivity in low dimensional structures. The value of complex ac conductivity was extracted from simultaneous measurements of the sound attenuation and velocity. The measurements were performed in the frequency range 17-300MHz, at temperatures down to 0.3K and in the magnetic fields up to 18T. Such measurements allowed to study, for example, mechanisms of conductivity in a dense array of SiGe quantum dots and localization of the 2D carries in GaAs/AlGaAs and Si/SiGe heterostructures in the ultraquantum limit. An extended list of coauthors will be presented during the presentation.

12:51PM Y37.00009 Effects of capture, escape and confinement on SAW-dragged photocurrents in a single QW, GODFREY GUMBS, Hunter College of CUNY, DANHONG HUANG, USAF Research Lab, MICHAEL PEPPER, Cavendish Lab of Univ. Cambridge, UK — A dual-plasma model is developed for studying the steady-state transport of SAW-dragged photocurrents of 1D confined-state carriers. This model includes the effects of the quantum confinement and the tunneling escape of SAW-dragged 1D carriers, as well as the effects of the inelastic capture of 2D continuous-state carriers and the space-charge field. The numerical results uncover a high photocurrent gain due to suppressed recombination of 1D carriers in a crossover region of the sample between an absorption strip and a surface gate. Based on a discrete model, responsibilities for the SAW-dragged photocurrents in a quantum well are calculated as functions of the gate voltage, photon flux, SAW power and frequency and temperature, respectively.

1:03PM Y37.00010 Evidence of Real-Space Transfer in Buried-Channel Ge$_x$C$_{1-x}$ Devices , EN-SHAO LIU, Microelectronic Research Center, University of Texas at Austin, DAVID KELLY, Texas Instruments, JOSEPH DONNELLY, EMANUEL TUTUC, SANJAY BANERJEE, Microelectronic Research Center, University of Texas at Austin — We present experimental evidence of real-space transfer (RST) in buried-channel Ge$_x$C$_{1-x}$ p-type metal-oxide-semiconductor field effect transistors (MOSFET) containing a Si cap layer. The output characteristics of these devices reveal a negative differential resistance (NDR) below 150K, at the onset of the saturation regime. This observation indicates a charge transfer from Ge$_x$C$_{1-x}$ layer into the Si cap at sufficiently large drain bias values. The lower hole mobility of the Si cap with respect to the Ge$_x$C$_{1-x}$, translates into a drain current reduction, hence the observed NDR. Our low-field, temperature-dependent mobility measurements indeed reveal a higher effective carrier mobility in the buried-channel Ge$_x$C$_{1-x}$ layer with respect to a Si-reference sample, which suggests that the observed NDR is caused by RST of holes from the Ge$_x$C$_{1-x}$ into the Si layer.

1:15PM Y37.00011 Tunable Channel Interference in an Aharonov-Bohm Ring , YIPING LIN, PEI-JUNG WU, KUAN TING LIN, J. C. CHEN, Dep. of Physics, National Tsing Hua University, Hsinchu, Taiwan, T. UEDA, S. KOMIYAMA, Dep. of Basic Science, University of Tokyo, Meguro-ku, Tokyo, Japan — We have investigated the Aharonov-Bohm effect in a quasi one-dimensional ring on a GaAs/Al$_{0.33}$Ga$_{0.67}$As heterostructure, which is defined by two metallic arc gates coupled to each branch of the ring. Each gate can be separately biased to uniformly squeeze the channel width of electrons, thereby externally tuning the transverse modes in the interference paths. The oscillatory magnetococonductance of the device is systematically studied by varying the number of channels in each path. We have observed the evidence of phase shifts in the magnetococonductance oscillations due to the suppression of the mode numbers on the ring path. Though the periodicity is not well resolved, qualitatively our data support the random phase shifts between the successive modes.

1:27PM Y37.00012 Energy Relaxation in the Bloch-Gruneisen Regime Probed by Weak Antilocalization (WAL) Measurements in GaN Heterostructures , HAILING CHENG, CAGLIYAN KURDAK, Physics Department, University of Michigan, NECMI BIYIKLI, JINQIAO XIE, HADIS MORKOC, Department of Electrical Engineering, Virginia Commonwealth University — Electron-phonon (e-p) interaction was investigated in wurtzite Al$_{0.15}$Ga$_{0.85}$N/AIn/GaN and Al$_{0.83}$In$_{0.17}$/N/AIn/GaN heterostructures with polarization induced two dimensional electron gases in the Bloch-Gruneisen regime. WAL and Shubnikov-de Haas measurements were performed on gali Hall bar structures at temperatures down to 0.3 K. With gate voltage, we cover a carrier density range from $3.41 \times 10^{12}$ cm$^{-2}$ to $4.92 \times 10^{12}$ cm$^{-2}$. Moreover, we used the WAL as a thermometer to measure the electron temperature $T_e$, as a function of the bias current. We find the power dissipated per electron $P_e$ is proportional to $T_e^3$ due to piezoelectric acoustic phonon emission by hot electrons. We calculated $P_e$ as a function of $T_e$ without using any adjustable parameters for both static and dynamic screening cases of piezoelectric e-p coupling. In the dynamic range of this experiment, the static screening case is expected to be applicable; however, our data are in better agreement with the dynamic screening case.

1:39PM Y37.00013 Bloch Oscillations and Saturation to a Steady-State Current of an Electron Gas in a Modulated Quantum-Wire Superlattice in a High Electric Field, S.K. LYO, Sandia National Laboratories, D. HUANG, Air Force Research Laboratory, W. PAN, Sandia National laboratories — We present rigorous theoretical results for the time-dependent and steady-state nonlinear DC current of an electron gas in a periodically modulated one-dimensional semiconductor quantum wire in a high electric field. The theoretical model considers electron-phonon and impurity scattering microscopically in the degenerate and the nondegenerate regime in a tight-binding model. The time-dependent oscillatory and saturation (i.e., steady-state) currents are studied as a function of the field, the radius of the wire, the elastic scattering rate, the lattice period, and the temperature. The radius controls the inelastic scattering rate. The distinctive roles of elastic and inelastic scattering for the current are contrasted and examined. Finally, we compare the results with those from an exact analytic formalism based on a relaxation-time model.

1Supported by National Science Council (Taiwan)

2Supported by the U.S. DOE under Contract No.DE-AC04-94AL85000.
the aeroelastic response of the flat plate is a function of Reynolds number. Also, the aeroelastic response of the flat plate influences the vortex shedding between a subsonic flow and a flexible flat plate. The results of the present analysis indicate that there is a strong fluid-structure coupling. It was observed that can be excited, causing damaging instabilities. In the present analysis, the dependence of vortex shedding on the aeroelastic response of a vertical flat plate in body locations determined by the forcing geometry; when the driving is strong, they wander over the flow domain and interact pairwise. By comparing the behavior of several base flows, we show that our methods are robust even for complex flow situations.

Supported by NSF-DMR-0405187.

11:27AM Y39.00002 ABSTRACT HAS BEEN MOVED TO SESSION D9 –

11:39AM Y39.00003 The dependence of vortex shedding on the aeroelastic response of a bluff body. MARCEL ILIE, Carleton University — Airflow over a vertical flat plate is investigated as a function of Reynolds number, using Large Eddy Simulation. It is generally known that the structure of the wake, behind a bluff body, exhibits very complex turbulent flow patterns. In many practical applications the bluff bodies are flexible structures and this characteristic enables them to respond to the aerodynamic loads. The fluid-structure interaction phenomenon is of critical importance due to the inheriting danger associated with the vortex induced vibrations. The periodic shedding of vortices may result in significant fluctuating loading on the body. When the shedding frequency is close to one of the characteristic frequencies of the body, the resonant oscillations of the body can be excited, causing damaging instabilities. In the present analysis, the dependence of vortex shedding on the aeroelastic response of a vertical flat plate in cross-flow is investigated. A CFD based algorithm, using Large Eddy Simulation, is developed for the investigation of a strong (two-way) aeroelastic coupling between a subsonic flow and a flexible flat plate. The results of the present analysis indicate that there is a strong fluid-structure coupling. It was observed that the aeroelastic response of the flat plate is a function of Reynolds number. Also, the aeroelastic response of the flat plate influences the vortex shedding.

VKS: a turbulent homogeneous dynamo with liquid sodium1, MICHAEL BERHANU, Ecole Normale Superieure — The magnetic field of the earth and of most astrophysical objects result from turbulent flows of electrically conducting fluids: the kinetic energy of the flow is converted into magnetic energy by dynamo effect. In September 2006 we observed this effect for the first time in a closed homogeneous turbulent flow of liquid sodium at very high Reynolds number in the Von-Karman Sodium (VKS). Despite the strong level of the fluctuations of the flow, we observed the growth and saturation of a stationary global mode of the magnetic field at the experiment’s characteristic length. Does turbulence act as noise or does it participate in the magnetic generation process? If we modify the global properties of the flow, we observe transitions between different magnetic field modes, going from stationary to oscillatory, and, near the frontiers between these modes, interesting dynamical behaviours occur, such as bursts and relaxations cycles. In particular we found a state with reversals of the magnetic field similar to those of the Earth recorded on geological time scale. These evolutions present some features of low dimensional chaos, compatible with the interaction between few modes. Finally we observe for the first time bistability from a stationary dynamo to an oscillatory one.

VKS collaboration: ENS, CEA Saclay, ENS Lyon.

12:03PM Y39.00005 Dynamical Phase Transitions and Scaling Laws in the Response of a Rhythmically Perturbed Neuron. JAN ENGELBRECHT, RENATO MIROLLO, Boston College — In order to explore how a local rhythm influences the timing of a neuron’s spikes, we study the dynamics of an integrate-and-fire model neuron with an oscillatory stimulus. The frustration due to the competition between the neuron’s natural firing period and that of the oscillatory rhythm leads to a rich structure of asymptotic phase locking patterns and ordering dynamics. The phase transitions between these states can be classified as either tangent or discontinuous bifurcations, each with its own characteristic scaling laws. The discontinuous bifurcations exhibit a new kind of phase transition that may be viewed as intermediate between continuous and first order, while tangent bifurcations behave like continuous transitions with a diverging coherence scale.

12:15PM Y39.00006 Correlations, fluctuations and stability of a finite-size network of coupled oscillators1, MICHAEL BUICE, CARSON CHOW, National Institutes of Health — The incoherent state of the Kuramoto model of coupled oscillators exhibits marginal modes in mean field theory. We demonstrate that correlations due to finite size effects render these modes stable in the subcritical case, i.e. when the population is not synchronous. This demonstration is facilitated by the construction of a non-equilibrium statistical field theoretic formulation of a generic model of coupled oscillators. This theory is consistent with previous results. In the all-to-all case, the fluctuations in this theory are due completely to finite size corrections, which can be calculated in an expansion in 1/N, where N is the number of oscillators. The N → infinity limit of this theory is what is traditionally called mean field theory for the Kuramoto model.

1Intramural Research Program of NIH/NIDDK.

12:27PM Y39.00007 Time-Shifts and Correlations in Synchronized Chaos. JONATHAN BLAKELY, NED CORRON, US Army RDECOM — We introduce a new method for predicting characteristics of the synchronized state achieved by a wide class of uni-directional coupling schemes. Specifically, we derive a transfer function from the coupling model that provides estimates of the correlation between the drive and response waveforms, and of the time shift (i.e., lag or anticipation) of the synchronized state. Notably, this approach does not require modeling or simulation of the full coupled system. To demonstrate the method, we compare its predictions to simulations of a variety of different coupled oscillator systems as well as to an experimental system of coupled chaotic electronic circuits. Finally, we show that the transfer function can be exploited to design novel coupling schemes that significantly improve the correlation and increase the maximum achievable time shift.
A linear reformulation of the Kuramoto model of self-synchronizing coupled oscillators. David Roberts, Los Alamos National Laboratory — This talk will present a linear reformulation of the Kuramoto model describing a self-synchronizing phase transition in a system of globally coupled oscillators that in general have different intrinsic frequencies. The reformulated model provides an alternative coherent framework through which one can analytically tackle synchronization problems that are not amenable to the original Kuramoto analysis. It allows one to 1) find an analytic solution for a new class of continuum systems and 2) solve explicitly for the synchronization order parameter and the critical point of the phase-locking transition for a system with a finite number of oscillators (unlike the original Kuramoto model, which is solvable implicitly only in the mean-field limit). It also makes it possible to probe the system’s dynamics as it moves towards a steady state. While this talk will cover only systems with global coupling, the new formalism introduced by the linear reformulation also lends itself to solving systems that exhibit local or asymmetric coupling.

Constructing almost invariant sets for multi-stable systems, Gabriele Migliorini, NCRG - Aston University - UK — We present a renormalization group study of two dimensional arrays of oscillators, with dissipative, short range interactions. We consider the case of non-identical oscillators, with distributed intrinsic frequencies within the array and study the steady-state properties of the system. In two dimensions no macroscopic mutual entrainment is found but, for identical oscillators, critical behavior of the Berezinskii-Kosterlitz-Thouless type is shown to be present. We then discuss the stability of (BKT) order in the physical case of distributed quenched random frequencies. In order to do that, we show how the steady-state dynamical properties of the two dimensional array of non-identical oscillators are related to the equilibrium properties of the XY model with quenched randomness, that has been already studied in the past. We propose a novel set of recursion relations to study this system within the Migdal-Kadanoff renormalization group scheme, by mean of the discrete clock-state formulation. We compute the phase diagram in the presence of random dissipative coupling, at finite values of the clock state parameter. Possible experimental applications in two dimensional arrays of microelectromechanical oscillators are briefly suggested.

The author acknowledge support from EPSRC.

Correlations of Coupled Logistic Maps, John Harrison, Richard Taylor, Gus Hart, Brigham Young University — Many systems in the world are non-linear and therefore often chaotic. Moreover, many systems influence or are influenced by other physical systems. That is, systems are often coupled to other systems. In an effort to uncover the fundamental issues of coupled systems, we have studied a system of coupled logistic maps. The logistic map, arguably the simplest chaotic system, shows unusual correlations when coupled to a second logistic map. We use a master–slave coupling, where the first map influences the second, but not the other way around. At low coupling strengths the correlations are complex but the two maps do not completely synchronize. At higher coupling strengths, the two maps “lock”, becoming synchronized. The value of coupling that causes the two maps to lock can be determined analytically. Intriguingly, at intermediate couplings strengths, periodic forcing by the master can result in chaotic behavior in the slave.

11:45AM Y40.00008 A computer simulation of polymer reversal inside a pore, Lei Huang, Dmitrii E. Makarov, University of Texas at Austin — Translocation of biopolymers through pores is implicated in many biological phenomena. Confinement within pores often breaks ergodicity on biological time scales by creating large entropic barriers to rearrangements of the chain. We study one example of such hindered rearrangement, in which the chain reverses its direction inside a long pore. Our goal is two-fold. First, we study the dependence of the polymer reversal timescale while the transmission factor, i.e., the ratio of the exact rate and the TST one, has a much weaker, power law dependence on the pore size and on the polymer length. Second, we examine the ability of simple theories, such as transition state theory (TST) and Kramers’ theory to quantitatively describe a transition in a system with a complex energy landscape. We find that one-dimensional TST using the polymer extension along the pore axis as the reaction coordinate adequately accounts for the exponentially strong dependence of the reversal rate on the pore radius $r$, and the polymer length $N$, while the transmission factor, i.e., the ratio of the exact rate and the TST one, has a much weaker, power law $r$ and $N$ dependence.

Refoldable Peptide Barrel – Carbon Nanotube Junctions, Alexey Titov, Boyang Wang, Petr Kral, University of Illinois at Chicago, PROF. KRAL’S RESEARCH GROUP TEAM — We design hybrid bio-nano-junctions formed by cylindrical peptide structures covalently attached to carbon nanotubes. The cylinders are composed of 5 pairs of antiparallel peptide strands that are “one-to-one” matched and covalently bonded through ester and amide bonds to the terminal C atoms in two (20,0) carbon nanotubes. The remaining terminal carbons in the CNTs are replaced by nitrogens, forming embedded quinoline-like structures. The used peptide strands are composed of charged amino acids that form cylindrical patterns with preferred stable configurations. By applying a torque to the nanotubes, we can reversibly fold and control the overall structure of the peptide barrels. The junctions might allow the collection and delivery of drugs and activation of biological molecules attached to them.

12:39PM Y39.00008 A linear reformulation of the Kuramoto model of self-synchronizing coupled oscillators, David Roberts, Los Alamos National Laboratory — This talk will present a linear reformulation of the Kuramoto model describing a self-synchronizing phase transition in a system of globally coupled oscillators that in general have different intrinsic frequencies. The reformulated model provides an alternative coherent framework through which one can analytically tackle synchronization problems that are not amenable to the original Kuramoto analysis. It allows one to 1) find an analytic solution for a new class of continuum systems and 2) solve explicitly for the synchronization order parameter and the critical point of the phase-locking transition for a system with a finite number of oscillators (unlike the original Kuramoto model, which is solvable implicitly only in the mean-field limit). It also makes it possible to probe the system’s dynamics as it moves towards a steady state. While this talk will cover only systems with global coupling, the new formalism introduced by the linear reformulation also lends itself to solving systems that exhibit local or asymmetric coupling.

Constructing almost invariant sets for multi-stable systems, Gabriele Migliorini, NCRG - Aston University - UK — We present a renormalization group study of two dimensional arrays of oscillators, with dissipative, short range interactions. We consider the case of non-identical oscillators, with distributed intrinsic frequencies within the array and study the steady-state properties of the system. In two dimensions no macroscopic mutual entrainment is found but, for identical oscillators, critical behavior of the Berezinskii-Kosterlitz-Thouless type is shown to be present. We then discuss the stability of (BKT) order in the physical case of distributed quenched random frequencies. In order to do that, we show how the steady-state dynamical properties of the two dimensional array of non-identical oscillators are related to the equilibrium properties of the XY model with quenched randomness, that has been already studied in the past. We propose a novel set of recursion relations to study this system within the Migdal-Kadanoff renormalization group scheme, by mean of the discrete clock-state formulation. We compute the phase diagram in the presence of random dissipative coupling, at finite values of the clock state parameter. Possible experimental applications in two dimensional arrays of microelectromechanical oscillators are briefly suggested.

The author acknowledge support from EPSRC.

Correlations of Coupled Logistic Maps, John Harrison, Richard Taylor, Gus Hart, Brigham Young University — Many systems in the world are non-linear and therefore often chaotic. Moreover, many systems influence or are influenced by other physical systems. That is, systems are often coupled to other systems. In an effort to uncover the fundamental issues of coupled systems, we have studied a system of coupled logistic maps. The logistic map, arguably the simplest chaotic system, shows unusual correlations when coupled to a second logistic map. We use a master–slave coupling, where the first map influences the second, but not the other way around. At low coupling strengths the correlations are complex but the two maps do not completely synchronize. At higher coupling strengths, the two maps “lock”, becoming synchronized. The value of coupling that causes the two maps to lock can be determined analytically. Intriguingly, at intermediate couplings strengths, periodic forcing by the master can result in chaotic behavior in the slave.

11:45AM Y40.00008 A computer simulation of polymer reversal inside a pore, Lei Huang, Dmitrii E. Makarov, University of Texas at Austin — Translocation of biopolymers through pores is implicated in many biological phenomena. Confinement within pores often breaks ergodicity on biological time scales by creating large entropic barriers to rearrangements of the chain. We study one example of such hindered rearrangement, in which the chain reverses its direction inside a long pore. Our goal is two-fold. First, we study the dependence of the polymer reversal timescale while the transmission factor, i.e., the ratio of the exact rate and the TST one, has a much weaker, power law dependence on the pore size and on the polymer length. Second, we examine the ability of simple theories, such as transition state theory (TST) and Kramers’ theory to quantitatively describe a transition in a system with a complex energy landscape. We find that one-dimensional TST using the polymer extension along the pore axis as the reaction coordinate adequately accounts for the exponentially strong dependence of the reversal rate on the pore radius $r$, and the polymer length $N$, while the transmission factor, i.e., the ratio of the exact rate and the TST one, has a much weaker, power law $r$ and $N$ dependence.

Refoldable Peptide Barrel – Carbon Nanotube Junctions, Alexey Titov, Boyang Wang, Petr Kral, University of Illinois at Chicago, PROF. KRAL’S RESEARCH GROUP TEAM — We design hybrid bio-nano-junctions formed by cylindrical peptide structures covalently attached to carbon nanotubes. The cylinders are composed of 5 pairs of antiparallel peptide strands that are “one-to-one” matched and covalently bonded through ester and amide bonds to the terminal C atoms in two (20,0) carbon nanotubes. The remaining terminal carbons in the CNTs are replaced by nitrogens, forming embedded quinoline-like structures. The used peptide strands are composed of charged amino acids that form cylindrical patterns with preferred stable configurations. By applying a torque to the nanotubes, we can reversibly fold and control the overall structure of the peptide barrels. The junctions might allow the collection and delivery of drugs and activation of biological molecules attached to them.
12:03PM Y40.00005 In vitro optical measurements of the interaction between human lung cells and single-wall carbon nanotubes, M. L. BECKER, J. A. FAGAN, J. CHUN, B. J. BAUER, E. K. HOBBIE, NIST — The intrinsic band gap fluorescence of individual semiconducting single-wall carbon nanotubes (SWNTs) stabilized with single-stranded DNA and deoxycholate surfactant is exploited to optically measure the interaction between human lung cells and length-fractionated SWNTs. Using near-infrared (NIR) fluorescence microscopy in microfluidic flow platforms, live human lung fibroblasts (IMR-90) are exposed to controlled quantities of length-sorted single wall nanotubes, and the cellular interaction and uptake of the SWNTs is optically monitored in real space-time. Cell mortality is shown to result from the uptake of shorter nanotubes and is correlated with both SWNT length and concentration. The NIR optical measurements are used to identify potential uptake mechanisms and quantify the kinetics of the interaction.

12:15PM Y40.00006 AFM and XPS Studies of Oligodeoxyribonucleotides associated with Single Walled Carbon Nanotubes, ROYA R. LAHJII, B. D. DOLASH, D. ZEMLYANOV, D. E. BERGSTRÖM, R. REIFENBERGER, Birck Nanotechnology Center, Purdue University — Oligodeoxyribonucleotide (ODN) disperse single wall carbon nanotubes (SCWNTs) in aqueous solution via sonication. By developing procedures that produce ODN:SWCNT hybrids uniformly dispersed in an aqueous solution, new biological applications will emerge. We have studied ODN T30:SCWNT hybrids that form after different preparation techniques. Deposition of the resulting ODN T30:SCWNT hybrids onto both insulating and conducting substrates have been studied. AFM under ambient conditions reveals localized features decorating individual SWCNTs having an approximate height consistent with the dimensions of single stranded T30 ODN. XPS confirmed the decorative features are ODN. Taking advantage of the ODN negative charge, we studied the deposition of ODN:SCWNT hybrids on Au substrates using electrophoretic deposition techniques. Electrodeposition has advantages since it does not require functionalization of ODN or the substrate prior to deposition. Applying a positive potential to the Au substrate can produce a uniform deposit of T30 ODN:SCWNT hybrids. The electrodeposited ODN:SCWNTs were further studied using AFM and XPS. [1] M. Zheng et al, Nat Mater 2003, 2, 338. [2] R. R. Lahiji et al, Small 2007, 3, 1912.

12:27PM Y40.00007 Atomic Scale Spectroscopy of Protein Active Sites, J.T. SAGE, Northeastern Univ., B.M. LEU, W. STURHAHN, E.E. ALF, Argonne Natl. Lab — We use nuclear resonance vibrational spectroscopy (NRVS) to investigate $^{57}$Fe embedded in protein matrices. Access to the complete spectrum of Fe vibrations allows experimental determination of effective local force constants. The stiffness reflects the force required to displace the probe nucleus with respect to its nearest neighbors and provides a direct probe of local structure. In contrast, the resilience describes the force required to displace the probe atom with neighboring atoms free to respond, and determines the thermal fluctuations of the Fe. We find that additional covalent links to the protein increase the resilience of the Fe site in cytochrome c as compared to myoglobin.

12:39PM Y40.00008 The Directed Assembly of Conducting Polymer Nanowires¹, BRENT FLANDERS, PREM THAPA, Oklahoma State University, RAY BAUGHMAN, NORMAN BARISCI, University of Texas at Dallas — The Directed Electrochemical Nanowire Assembly (DENA) technique is a single-step approach to fabricating metallic nanowires and interconnecting them with external circuitry or other objects. Here we expand this technique to include the growth of non-metallic wires. From aqueous pyrrole solutions, individual wires were grown from the tip of one electrode across a 30 µm electrode gap and into contact with the tip of the other electrode. Energy dispersive spectroscopy is used to show that the wires are composed of doped polypyrrole. The conductance of these nanowires will be discussed, as well as the interfacing of DENA nanowires with biological cells for cell stimulation studies.

¹This research was supported by funding from the National Science Foundation (PHY-646966).

12:51PM Y40.00009 Directed Electrochemical Nanowire Assembly¹, PREM THAPA, BRENT FLANDERS, Oklahoma State University — Directed Electrochemical Nanowire Assembly (DENA) technique is a single-step approach to fabricating metallic nanowires and interconnecting them with external circuitry. We have previously shown that these are near single crystalline metallic nanowires and that they interconnect with on-chip electrodes with very small contact resistances. Here we discuss the user-directed growth of these nanowires up to inter-electrode targets, such as biological cells. Recent results on the delivery of small voltages to these targets will be discussed, as well.

¹This research was supported by the National Science Foundation (PHY-646966).

1:03PM Y40.00010 Electrochemical measurement of DNA in a nanofluidic channel, CHIH-KUAN TUNG, Dept of Physics, Princeton University, ROBERT RIEHN, North Carolina State University, ROBERT H. AUSTIN, Dept of Physics, Princeton University — The elongation of genomic length DNA in confining nanochannels is not only a fascinating exercise in polymer dynamics, but also is of great interest in biotechnology because the elongation of the confined molecule is directly proportional to the actual length of the molecule in basemaps. We will present a way to construct nanochannels using sacrificial PMMA ebeam lithography and to measure non-immobilized DNA molecules inside such a channel electrochemically. This kind of measurements can lead us to fast and precise electronic length measurement, which will open the door to a number of important areas in genomics such as gene exchange and evolution dynamics of single cells.

1:15PM Y40.00011 A nanofluidic lateral Coulter counter, YONG SUN, JUNHAN PAN, ROBERT RIEHN, North Carolina State University — Optical detection has been the mainstay of detection in many micro-and nanofluidic systems. However, the need for labeling and alignment of detectors or registration of images has slowed transition to application and increased cost. On the other hand, when traditional Coulter counters that detect along the axis of a fluidic channel are integrated with nanofluidics on a chip, leakage and limited resolution often present problems. For that reason, we are developing an electronic detection mechanism that is based on the impedance change of an electrode pair that is laterally integrated with a nanochannel. We will present detection of 50 nm polystyrene beads, and will discuss possible applications in the detection of biological molecules such as DNA.

1:27PM Y40.00012 On the virus capsid assembly and encapsulation of foreign materials, CHAO CHEN, Ph.D. Candidate, Chemistry Department, Indiana University, BOGDAN DRAGNEA, Assistant Professor, Chemistry Department, Indiana University, CHENG KAO, Professor, Department of Biochemistry and Biophysics, Texas A&M University, ADAM ZLOTNICK, Associate Professor, Biochemistry & Molecular Biology, Health Sciences Center, the University of Oklahoma, BOGDAN DRAGNEA TEAM, C. CHENG KAO COLLABORATION, ADAM ZLOTNICK COLLABORATION — Icosahedral virus capsids are one of the simplest biological structures, yet poorly understood from a molecular physics point of view, e.g., the paradox between its stability and flexibility, its interaction with the virus genome, and its assembly thermodynamics and kinetics. In the hope of elucidating these problems, we have created a study platform based on virus-like particles (VLPs) – inorganic nanoparticles encapsulated inside icosahedral virus capsids in place of their genomic core. These nanoparticles were successfully incorporated when coated with carbonate-terminated poly-ethyleneglycols, implying a dominating electro-static interaction between the virus capsid and the core. The nano-particle size determines the T number of the icosahedral cage and the efficiency of encapsulation. The current work seeks to understand the mechanism of capsid assembly process using VLP as a model system. Empty capsid assembly kinetics has been also studied for comparison. A simplified kinetically limiting model based on a previously reported master equation model is proposed.
1:39PM Y40.00013 Assembly and Characterization of NanoComplexes: Quantum Dot Encapsulated Liposomes, ANGELA HIGHT WALKER, EMREN ESENTURK, PETER YIM, JEESEONG HWANG, Physics Laboratory, National Institute of Standards and Technology (NIST) — Liposome complexes have received significant attention for a variety of biochemical and biomedical applications including drug targeting and drug delivery and tumor imaging and diagnostics. Semiconductor nano-crystals, also known as quantum dots, are now beginning to be used in similar biochemical experiments. Like fluorescent dyes, these quantum dots have the ability to reliably fluoresce at pre-engineered wavelengths. However, these nano-crystals have lifetimes significantly longer comparable to fluorescence dye counterparts. We have successfully encapsulated approximately 10nm CdSe nano-crystals inside approximately 100nm liposomes and studied the resulting complex using fluorescence resonance energy transfer (FRET) microscopy. Further studies were performed using transmission electron microscopy (TEM) showing the details of the encapsulation, and Raman spectroscopy to examine their structural details. Our nano-manufactured quantum dot liposome complexes do not bleach over periods of hours and are general enough to allow the addition of drugs targeted for the vectored cells thus offering the ability to both image and medicate simultaneously over a long period of time.

1:51PM Y40.00014 Selective Cell Growth on Fibronectin-Carbon Nanotube Hybrid Nanosstructures, SEON NAMGUNG, SUNG YOUNG PARK, BYUNG YANG LEE, MINBAEK LEE, Department of Physics and NANO Systems Institute, Seoul National Univ., Korea, JWA-MIN NAM, Department of Chemistry, Seoul National Univ., Korea, SEUNG-HUN HONG, Department of Physics and NANO Systems Institute, Seoul National Univ., Korea — Carbon nanotubes (CNT) have been considered a promising material for biological applications including biosensors, therapeutic application, and nano-structured scaffolds. However, there are still controversies associated with toxicity and biocompatibility of CNTs on live cells. Here, we report general strategy to functionalize CNTs with cell adhesion molecules (fibronectins) for selective and stable adhesion of cells on CNTs. Interestingly, more fibronectins were adsorbed and activated on CNTs rather than on hydrophobic self assembled monolayers (SAMs) or bare substrates (SiO$_2$). We demonstrate the functionality of fibronectins on CNTs with immunofluorescence and molecule-level force measurement study using atomic force microscopy (AFM). These fibronectin-CNT hybrid nanostructures were successfully applied to attract cells selectively onto predefined regions on the substrate. Our strategy was generally available on various cell types including mesenchymal stem cells, KB cells, and NIH3T3 fibroblast cells (Advanced Materials 19, 2530-2534 (2007)). We will also discuss about its impacts on cell biology combined with CNTs.

2:03PM Y40.00015 Large-Scale ‘Linker-Free Assembly’ of SWCNT-Based Biosensor Arrays, DONGHEE SOHN, BYUNG YANG LEE, SEUNGHUN HONG, Department of Physics and NANO Systems Institute, Seoul National University, Seoul, Korea — Biosensors based on single-walled carbon nanotubes (swCNTs) have received a great deal of attention due to their potential applications such as genotyping, disease diagnosis, food analysis, etc. However, a lack of reliable mass-production method for such swCNT-based biosensor has been holding back their practical applications. One promising mass-production method for such swCNT-based biosensor arrays can be ‘linker-free assembly’ process (Nature Nanotechnology 1, 66 (2006)), where non-polar patterns guide the ‘selective assembly’ and ‘precision alignment’ of carbon nanotubes on bare substrates without using any external forces such as liquid flow, etc. We used this method to fabricate large-scale assembly of swCNT-based integrated devices on virtually general substrates including SiO$_2$, Si, Al, Au, etc. To utilize swCNT devices for biosensors, we functionalized swCNT devices on SiO$_2$ with receptor biomolecules such as enzyme L-glutamate oxidase or biotin. And then, we could detect the target biomolecules (L-glutamate or streptavidin, respectively) with high sensitivity and selectivity by monitoring the conductance change of swCNT junctions in aqueous environment. These studies provide biological implications on neurotransmitters and proteins onto swCNT patterned surface.